

A CALCULATIONAL MODEL FOR CONDENSED STATE DIFFUSION
CONTROLLED FISSION PRODUCT ABSORPTION
DURING FALLOUT FORMATION
OCD Work Unit # 3111A -- GA

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GENERAL ATOMIC

DIVISION OF GENERAL DYNAMICS

GA-7598

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by

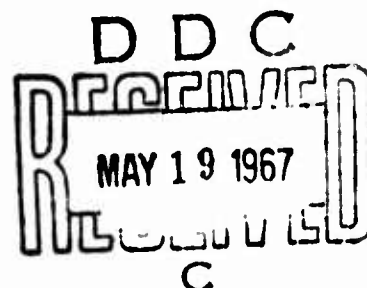
R. F. Korts and J. H. Norman

Performed for
Office of Civil Defense
Secretary of the Army
Department of Defense, 20301
under

Contract N0022866C0403

through the

**U.S. Naval Radiological Defense Laboratory
San Francisco, California 94135**



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The FORTRAN IV computer code for the UNIVAC 1108 described herein is as it existed on 12/1/66. The code has been in continuous development for 1 year and in its presented form has been applied successfully by General Atomic to the kind of problems discussed later in this report. However, the development and improvement of the code are being continued, so that duplication of results (or even close agreement) between problems run with the code as published and the code as it existed either before or after this time is not necessarily to be expected.

General Atomic has exercised due care in preparation, but does not warrant the merchantability, accuracy, and completeness of the code or of its description contained herein. The complexity of this kind of program precludes any guarantee to that effect. Therefore, any user must make his own determination of the suitability of the code for any specific use, and of the validity of the information produced by use of the code.

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ABSTRACT

A program is presented to compute fallout fission product absorption in an expanding, cooling, uniform field of gas and fallout particles where the rate of fission product absorption is controlled by fission product surface concentrations as given by Henry's law constants and diffusion of these fission products into the fallout particles. The calculations are made a nuclide chain at a time, employing nuclear device and fission product parameters. Program output includes average concentration versus particle size for each absorbed fission product at a preselected lower temperature and the amount of that fission product in the gas phase, with an option for the calculation of fission product radial profiles versus particle size. As a demonstration of this model, an initial computer study of fallout formation phenomenology is presented.

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SUMMARY

The computer code described in this report represents a model of fallout fission product absorption, the fallout particles being distributed uniformly in a cooling, expanding field of gas. Rates of fission product absorption are governed by fission product surface concentrations as given by Henry's law constants and by diffusion into the fallout particles. It is assumed that the particles neither agglomerate nor convect fission products during the time stepped calculational portion of the program. The absorption of fission products is considered for one decay chain at a time using detonation yields, initial fission product yields, half-lives, Henry's law constants, concentration independent diffusivities, and a fallout particle size versus quantity distribution. Output consists of surface concentration versus temperature for each absorbed fission product, average concentration versus particle size at a final lower temperature, and the amount of that fission product remaining in the gas phase. Optionally, radial profiles of fission product concentration versus particle size at this temperature are calculated.

Fission product distribution for mass chains 95 and 137 in fallout using this code are described. One of the important findings derived from these computer studies is an understanding of how this model considers fractionation to vary with fallout particle size distribution.

1. INTRODUCTION

Since the phenomenological discovery of fractionation of fission product elements in recovered fallout, the importance of the chemical properties of the fission products and fallout particles to the description of fallout formation has been recognized. In his treatise on fallout, Miller⁽¹⁾ has attempted to synthesize fractionation effects by allowing fission products to equilibrate with fallout until they have cooled to 1400°C and, thereafter, to surface condense on the fallout. This scheme has been considered an oversimplification and phenomenologically unsatisfactory. General Atomic has taken the position that condensed state diffusion of fission products in glassy silicate fallout particles can be considered to control the rate of fission product absorption. This report is a description of a calculational program written in FORTRAN IV for the UNIVAC 1108 in which the surface of fallout is considered to be in equilibrium with the gas phase, but bulk fallout phase absorption of fission products is diffusion controlled. In addition, fallout formation information derived from some computer experiments employing this model is presented in Appendix B.

2. GENERAL DESCRIPTION

The problem consists of determining concentrations of radioactive isotopes in fallout particles. Absorption of fission products is considered a decay chain at a time where a chain consists of a number of isotopes generally of the same mass. The last isotope in the chain is assumed to be stable for the time periods being considered. The fallout particles are assumed to be non-agglomerating, internally non-convecting, refractory, spherical glassy silicate bodies of various sizes uniformly distributed throughout a uniform temperature-concentration cloud of particles, air, and fission products. Immediately after the detonation takes place, temperatures are very high and chemistry in the cloud is unimportant. However, at a time when the cloud has cooled sufficiently to consider chemistry, this program can be applied. From this point, as time progresses (and the temperature of the cloud further decreases) the isotopes are assumed to surface condense according to Henry's law and subsequently to be diffused into the particles. Concurrently, the isotopes decay from one to another at rates dependent upon their respective half-lives. At a sufficiently low temperature, the diffusion process is considered to terminate leaving the isotopes distributed among and within the particles in some manner. The purpose of the program is to describe that distribution in terms of surface concentrations, average concentrations, and concentrations throughout the particles (profiles). To find these various concentrations, it suffices to calculate gas and condensed phase mass balances in which surface concentrations of each isotope are determined as a function of time.

Time-temperature stepping is employed in the program, and mass balances are determined at each time step. In order to determine the mass

balances, it is necessary to use input nuclear cloud parameters and chemical information. Time scaling functions for temperature and for cloud volume and a fallout mass representation are employed according to Miller⁽¹⁾ but can be changed to fit other circumstances. Fission product yields can be taken from Crocker,⁽²⁾ and fission product decay rates can be taken from Crocker, Scheidt, and Connors.⁽³⁾ Henry's law constants for this program have been presented by Norman.⁽⁴⁾ A similar report on diffusion coefficients for this program is planned.

Surface concentrations are obtained directly from the mass balance calculations. Other output parameters are calculated from the surface concentration values and the degree of diffusion that has been calculated. The computation of concentration profiles of the various sized particles at a final temperature is optional. Another option allows calculation of late distributions at such a time that all remaining gaseous short-lived isotopes have decayed and condensed. In this option, it is assumed that the isotopes are deposited on the particles according to surface area.

Surface concentrations are calculated at a finite number of points assuming that an actual time-temperature distribution can be closely approximated by a step function as shown in Fig. 1. The exact nature of this step function depends on the starting, final, and incremental temperatures (see Section 4.1, item 4). Thus, all temperature (and time) dependent quantities are assumed to be step functions as well; in particular, volumes and diffusion constants and Henry's law constants for each isotope remain constant for each temperature interval. Fission product surface concentrations are also assumed constant during any time interval.

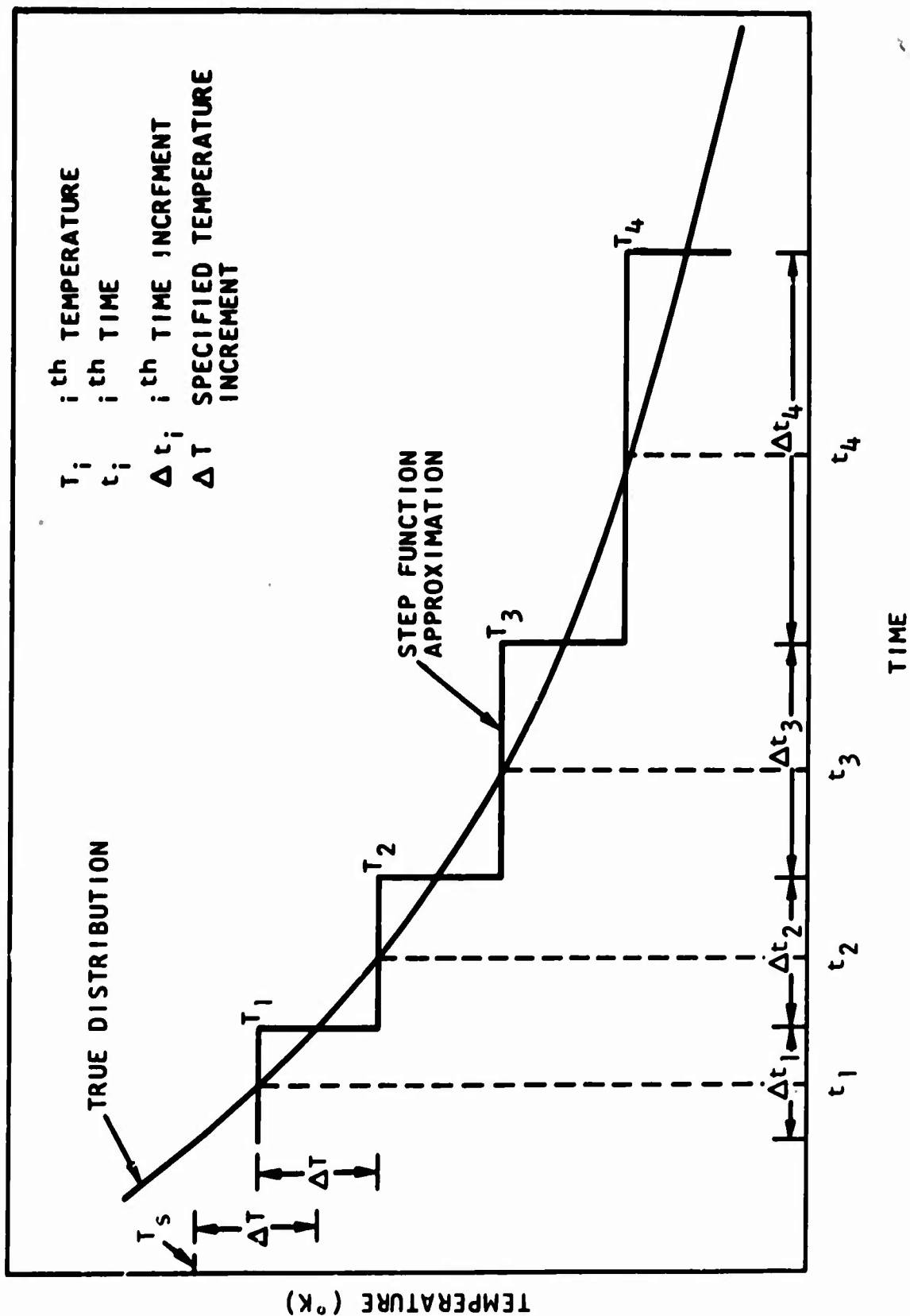


Fig. 1 -- Step function approximation to time-temperature distribution

3. METHOD

To determine the surface concentration of a given isotope at some temperature, the surface concentrations of that isotope and all its precursors at all preceding temperatures must be employed, since some fraction of each precursor will decay into the next isotope and previous surface concentrations will affect the total surface concentration at the specified temperature. We start by assuming that all of the fission products are uniformly distributed throughout the cloud at some sufficiently high temperature. To find surface concentrations at the first temperature, the following expression is used:

$$\frac{C_{i1} V_1 M_i H_{i1}}{RT_1} + C_{i1} \sum_{s=1}^P D_{i11}^{(s)} w_s = Y_{i1} \quad (1)$$

- where C_{i1} = surface concentration (g/g)* of isotope i at time t_1 (sec)
 V_1 = volume of nuclear cloud at time t_1 (liters)
 M_i = molecular weight of isotope i (g/mole)
 H_{i1} = Henry's law constant for isotope i at time t_1 (atm/g/g)
 R = ideal gas constant (liter atm/°K mole)
 T_1 = temperature at time t_1 (°K)
 Y_{i1} = yield, or total amount of isotope i , available at time t_1 (g)
 w_s = weight of soil (g) contained in particle size fraction s of radius r_s (cm)
 $D_{i11}^{(s)}$ = solution of the diffusion equation as if diffusion had taken place at a constant surface concentration C_{i1} (see Section 4.3) for particle of s^{th} radius, with the $\delta_{i1}\Delta t_1$ term for isotope i assumed constant during Δt_1 (δ_{i1} is the pertinent diffusion coefficient (δ in cm^2/sec)). The diffusion coefficients are assumed to be concentration independent.

*Suggested self-consistent units.

The Y_{i1} value is computed by considering the decay of isotopes and the H_{i1} value is computed from characteristics of the isotope and temperature (see Section 4. 1).

The first term on the left of Eq. (1) represents the amount of isotope i in the gas phase at time 1. The second term is the amount in the solid, or condensed, phase. For each s ,

$$D_{i11}^{(s)} = \frac{\bar{C}_{i1}^{(s)}}{C_{i1}}$$

for the s^{th} particle size, where $\bar{C}_{i1}^{(s)}$ is the average concentration during time t_1 . Thus

$$\begin{aligned} C_{i1} \sum_{s=1}^p D_{i11}^{(s)} w_s &= C_{i1} \sum_{s=1}^p \frac{\bar{C}_{i1}^{(s)} w_s}{C_{i1}} \\ &= \sum_{s=1}^p \bar{C}_{i1}^{(s)} w_s \end{aligned}$$

It should be noted that in this program an approximation system is used in representing the decay of fission products. During the time intervals used, a fission product is assumed to decay to one and only one product. Thus, decay is not treated as a dynamic process but as a discrete process occurring only at the end of a time step period. A nearly correct fission-product distribution is obtained at the initiation of the program by stepping the time in many small increments to this initial time after detonation. The time increments then become governed by the temperature increments. This system will cause some deviation from an exact decay solution but, generally, will only alter the final answers in a negligible fashion. Of course, as the temperature increment approaches zero, the decay system will approach the theoretical limit.

To find surface concentrations at the second temperature, the expression is

$$\begin{aligned}
& \frac{C_{i2} V_2 M_i H_{i2}}{RT_2} + C_{i1} \exp(-k_i \Delta t_1) \sum_{s=1}^P D_{i,1,2}^{(s)} w_s \\
& + C_{(i-1)1} [1 - \exp(-k_{i-1} \Delta t_1)] \sum_{s=1}^P D_{(i-1),1,i,2}^{(s)} w_s \\
& + \{C_{i2} - C_{i1} \exp(-k_i \Delta t_1) - C_{(i-1)1} [1 - \exp(-k_{i-1} \Delta t_1)]\} \sum_{s=1}^P D_{i,2,2}^{(s)} w_s = Y_{i2}
\end{aligned} \tag{2}$$

The terms on the left side of Eq. (2) can be explained as follows:

1. The first term is due to the amount of isotope i still in the gas phase.
2. The second term is due to the amount of i surface condensed associated with time t_1 decaying for Δt_1 and being diffused for $\delta_{i1} \Delta t_1 + \delta_{i2} \Delta t_2$.
3. The third term is due to the amount of isotope $i-1$ (the immediate precursor at t_1 of i) surface condensed at time t_1 decaying into i and being diffused as $i-1$ during time Δt_1 and as i during time Δt_2 .
4. The fourth term represents the amount of i being diffused within the particles as the result of the surface concentration increment caused by the temperature-time-volume increment.

The D 's are further defined in Appendix A.

It is apparent that as time is increased, the number of terms in the expression for C_{iN} becomes quite large. In fact, it can be shown (Appendix A) that if there are $n-1$ predecessors to an isotope, the number of terms required to find C_{iN} is

$$2^N - 1 \quad \text{if } N \leq n$$

and

$$\sum_{k=0}^{n-1} \left(\sum_{j=n}^{N-1} \binom{j}{k} \right) + 2^n - 1 \quad \text{if } N > n \quad (3)$$

plus additional terms for the gas phase contribution and yields.

The general expression for surface concentration can be written as

$$C_{iN} \frac{M_i V_N H_{iN}}{RT_N} + A_{iN} = Y_{iN} \quad (4)$$

where A_{iN} consists of the number of terms described by Eq. (3). Each term of A_{iN} is of the form

$$C_{(i-r)(N-j)} (\text{decay term}) \sum_{s=1}^P (D_{(1)} - D_{(2)})^w_s \quad (5)$$

where $0 \leq r \leq i-n+1$

$$0 \leq j \leq N-1$$

The decay term depends on the position of the isotope $i-r$ in the chain and on the time. $D_{(1)}$ and $D_{(2)}$ are diffusion terms which also depend on the position and time. (See Appendix A for details.)

Once surface concentrations have been found for all times, it remains to compute average concentrations and concentrations at various radii within the particles. Average concentrations can be obtained by mathematically combining concentration increments according to an additivity rule, as explained in Appendix A. Concentrations at any point within a particle can be found in an analogous way using relationships given by Crank. ⁽⁵⁾

4. SUBPROGRAM DESCRIPTIONS

This section describes each of the FORTRAN IV subroutines used by this code. Most of the variables used are stored in one of the common blocks described in Table 1.

4. 1. SUBROUTINE INITAL

This routine reads the data cards for each calculation and prepares the input data for the main program. The flow is in approximately the order described below.

1. Read input cards. The following information is read for each calculation with the internal variable name indicated in each case. (See Appendix C for card formats.)
 - a. Length of the chain, LC (≤ 6)
 - b. Yield of device used for calculating fission product yields (in kilotons TNT), YKT
 - c. Yield of device used for calculating the time-temperature distribution and the cloud volume (in kilotons TNT), BKT
 - d. For each isotope in the chain:
 - (1) Chemical symbol, NAME
 - (2) Molecular weight (in g/mole), WMOL
 - (3) Initial yield (in atoms/ 10^4 fissions), YI
 - (4) Half-life (in seconds), HL
 - (5) Constants used in calculating Henry's law constants and diffusion coefficients (see item 8), DC1, DC2, HC1, and HC2
 - e. Starting temperature, final temperature and incremental temperature (in $^{\circ}\text{K}$), HTMP, ETMP, and TEMPV (also referred to as T_s , T_f , and ΔT)

TABLE I
VARIABLES IN COMMON BLOCKS

Variable	Dimensions	Description
BLANK Common: Contained in NORMAN, BCALC, INITIAL		
YLD	(6, 40)	Yield of each isotope at each time step
NAME	(6)	Chemical symbol of each isotope
WMOL	(6)	Molecular weight of each isotope
DFC	(6, 40)	Diffusion coefficients of each isotope at each time step
HEN	(6, 40)	Henry's law constants for each isotope at each time step
AK	(6)	Exponential constant associated with each half-life
R	(30)	Radius of each particle size
WT	(30)	Weight of soil in each particle size
VOL	(40)	Volume of the cloud at each time step
T	(40)	Time increments
TEMP	(40)	Temperatures at each time step
ATM	(40)	Times at each step
SING: Contained in NORMAN, FINAL, BCALC, INITIAL		
LC	(1)	Length of chain
IR	(1)	Number of particle sizes
NTOT	(1)	Number of time steps
NCS1	(1)	Case identification
NCS2	(1)	Case identification
TWT	(1)	Total mass of soil
ILG	(1)	Flag: if = 0, do not do FINAL calculation if \neq 0, do FINAL calculation
IDPTH	(1)	Number of radii used for profile calculations
Q	(11)	Relative radii for profile calculations
B1: Contained in NORMAN, BCALC, DELTA		
DCY	(6, 40, 40)	Array of decay constants for each isotope from each time step to each other
WN	(6, 40)	Array of concentration ratios times weights for each isotope at each time step
INLOOP: Contained in NORMAN, BCALC, DELTA		
L	(1)	Subscript of isotope presently under consideration

- f. Number of particle sizes, IR (≤ 30)
 - g. For each particle size, its radius (in cm) and the fraction of soil contained in particles of that size, R, PW
 - h. The total mass of soil (in g/KT), TWGT
2. Check starting temperature. If the starting temperature is so high that all the fission products are uniformly distributed throughout each particle, that temperature is lowered by one increment and the procedure is repeated until a temperature is reached where this is not the case. Calculations are initiated after stepping back one temperature increment or to the starting temperature. To accomplish this, a D for the largest particle radius is found for each isotope at an initial time step. A D of 1 implies that an isotope is uniformly distributed throughout all particles. If $D = 1$ for all isotopes and particle sizes, the process is not yet diffusion controlled; thus, if

$$\sum_{i=1}^{LC} D_i = LC ,$$

all D's are unity. (Note that $D \leq 1$.) If this is satisfied, the temperature is reduced and the procedure is repeated.

3. Calculate w_s , the weight of soil in each particle size:
 $w_s = TWT \cdot PW_s$, where $TWT = TWGT \cdot BKT$.
4. Calculate the time-temperature distribution. Using the formula⁽²⁾

$$T = 4.66 \times 10^3 (BKT)^{-0.010} \exp(-0.546(BKT)^{-0.373} t) = f(t) , \quad (6)$$

times and incremental times are calculated to correspond to each specified temperature. The temperatures are calculated from

$$T_n = T_s - \left(\frac{2n - 1}{2} \right) \Delta T ,$$

and the times such that

$$T_n = f(t_n) .$$

Δt_n is defined by

$$\Delta t_n = f^{-1}\left(T_n + \frac{\Delta T}{2}\right) - f^{-1}\left(T_n - \frac{\Delta T}{2}\right) \text{ (see Fig. 1) } . \quad (7)$$

5. Convert initial yields, Y_i , to grams.

$$Y_i(g) = Y_i \cdot \text{WMOL} \cdot YKT \cdot 2.3410261 \times 10^{-5}$$

6. Find the quantities k_i . These quantities are used to calculate decay coefficients where

$$d_{inm} = \exp[-k_i(\Delta t_n + \Delta t_{n+1} + \dots + \Delta t_m)] \quad m > n$$

$$= \exp(k_i \Delta t_n) \quad m = n$$

$$= 1 \text{ (a computational aid)} \quad m < n$$

and

$$k_i = \frac{\ln(2)}{HL_i} .$$

7. Calculate yields at t_s where

$$t_s = f^{-1}(T_s) .$$

Yields at t_s are approximated by the following scheme:

Let $\Delta h = \min(HL)/10$ when $\min(HL)$ is the minimum half-life in the chain

Let $\tau_n = n(\Delta h)$, and let $i-1$ specify the precursor of isotope i . Then,

$$Y_i(\tau_1) = Y_i(0) \exp(-k_i \Delta h) + Y_{i-1}(0) [1 - \exp(-k_{i-1} \Delta h)] \quad (8)$$

\vdots

$$Y_i(\tau_n) = Y_i(\tau_{n-1}) \exp(-k_i \Delta h) + Y_{i-1}(\tau_{n-1}) [1 - \exp(-k_{i-1} \Delta h)] \quad (9)$$

Equation (9) is repeated for all n and i until n is such that $\tau_{n+1} > t_s$. For the last step, Δh is changed such that $\Delta h = t_s - \tau_n$ and Eq. (9) is repeated. If the original $\Delta h \geq t_s$, Δh is set equal to t_s and only Eq. (8) is used.

8. Calculate diffusion coefficients and Henry's law constants. The expressions⁽⁴⁾

$$\log(H_{in}) = HC1_i - HC2_i / T_n \quad (10)$$

and

$$\log(\delta_{in}) = DC1_i - DC2_i / T_n \quad (11)$$

are used to find δ and H for all isotopes and temperatures.

9. Volumes are computed for all temperatures using the expression⁽³⁾

$$V_n = \left\{ 5.69 \times 10^2 (BKT)^{1/3} \exp[0.17(BKT)^{-0.373} t_n] \right\}^3 \frac{4\pi}{3}$$

10. Input and computed quantities are printed. Input is actually printed as it is read and calculated quantities as they are calculated. (See Appendix D for sample printout.)

4.2. MAIN ROUTINE (NORMAN)

The main routine has three basic functions:

1. Setup and initial calculation of arrays needed (such as yields and decay coefficients) for the main loop.
2. Execution of the main loop which finds surface concentrations, average concentrations, and profiles.
3. Writing out of results.

4.2.1. Setup and Initial Calculations

The main routine starts by calling subroutine INITAL, which supplies it with necessary input data. Next it computes the array of decay coefficients, d_{inm} , as defined in Section 4.1, item 6; the array of

yields Y_{in} , where Y_{in} is the yield of isotope i at time n ; and the arrays UN and WN. The yields are found by using Eq. (8), Section 4.1, item 7, modified as

$$Y_{in} = Y_{i,n-1} d_{i,n-1,n-1} + Y_{i-1,n-1} (1 - d_{i-1,n-1,n-1})$$

The UN^* and WN arrays are defined by

$$UN_{ins} = E(\delta_{in} \Delta t_n, r_s)$$

$$WN_{in} = \sum_{s=1}^p UN_{ins} w_s$$

where δ_{in} = diffusion coefficient of isotope i at time t_n

Δt_n = n^{th} time interval

r_s = radius of s^{th} particles

w_s = weight of soil in the s^{th} particle size

$E(\delta_{in} \Delta t_n, r_s)$ = solution of diffusion equation for sphere of radius r_s and $\delta_{in} \Delta t_n$ term

Finally, the surface concentrations are calculated for each isotope at time t_1 by the relation

$$C_{i1} \left(\frac{WMOL_i H_{i1} V_1}{RT_1} + WN_{i1} \right) = Y_{i1}$$

4.2.2. Main Loop[†]

The following steps are taken in the main loop for each isotope and each time:

1. Find the terms due to decay of this isotope from previous times.
2. For each precursor of this isotope at each preceding time, find all possible paths for decay, and for each such path find a diffusion term (see Section 4.8) and a decay term (see Section 4.7).

* $UN_{ins} = D_{inn}^{(s)}$
[†] See Fig. 2

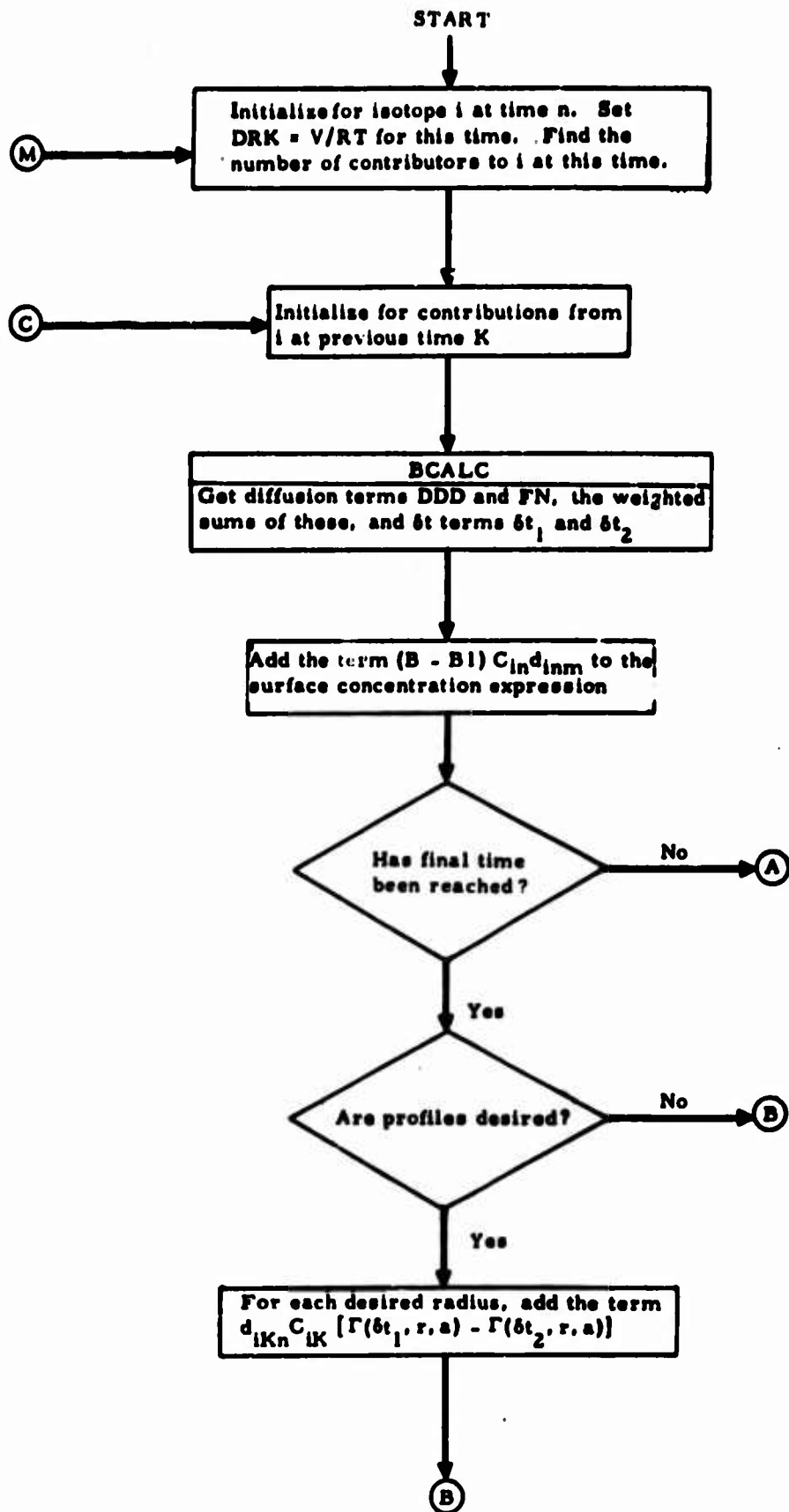


Fig. 2--Flow chart, main loop NORMAN (Sheet 1 of 5)

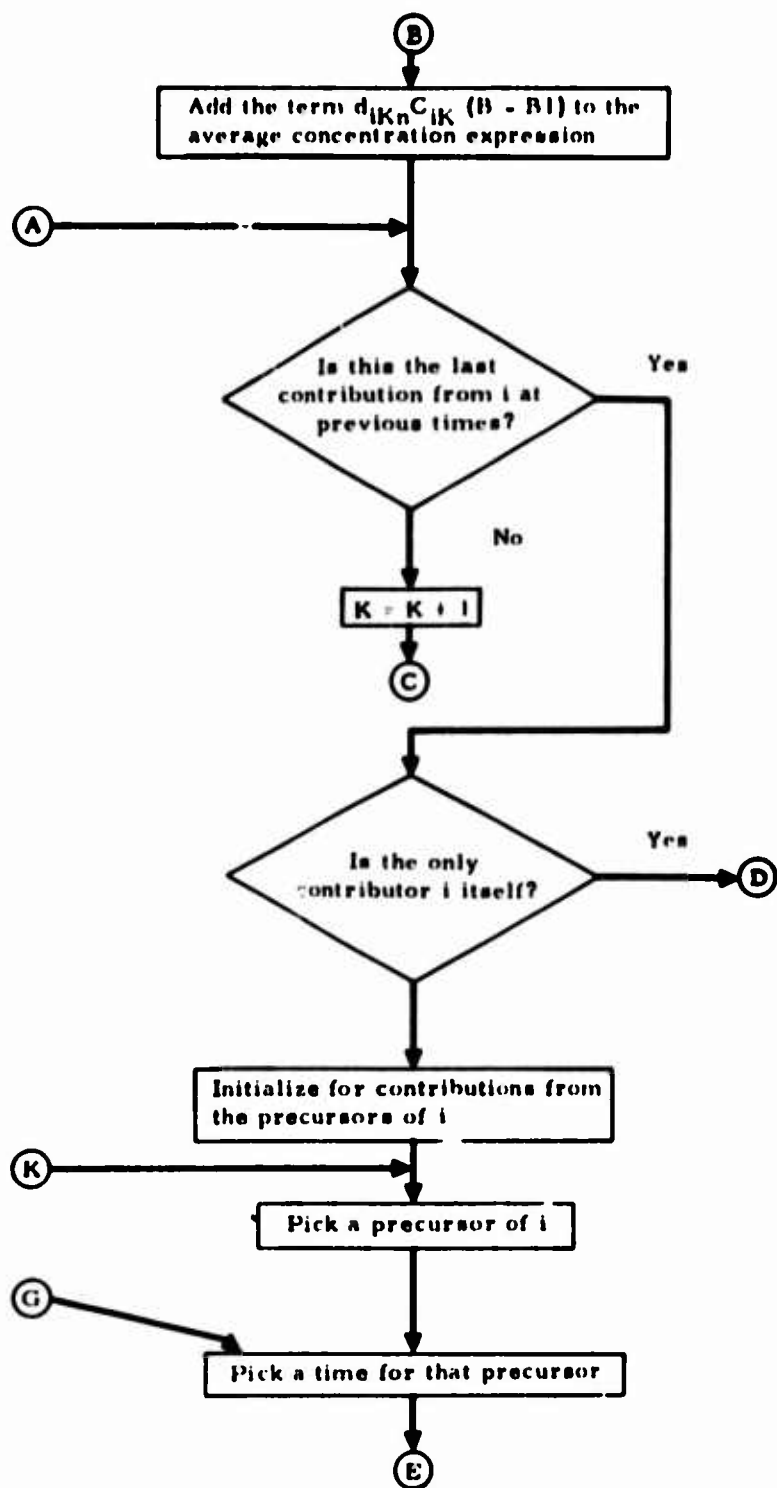


Fig. 2-- Flow chart, main loop NORMAN (Sheet 2 of 5)

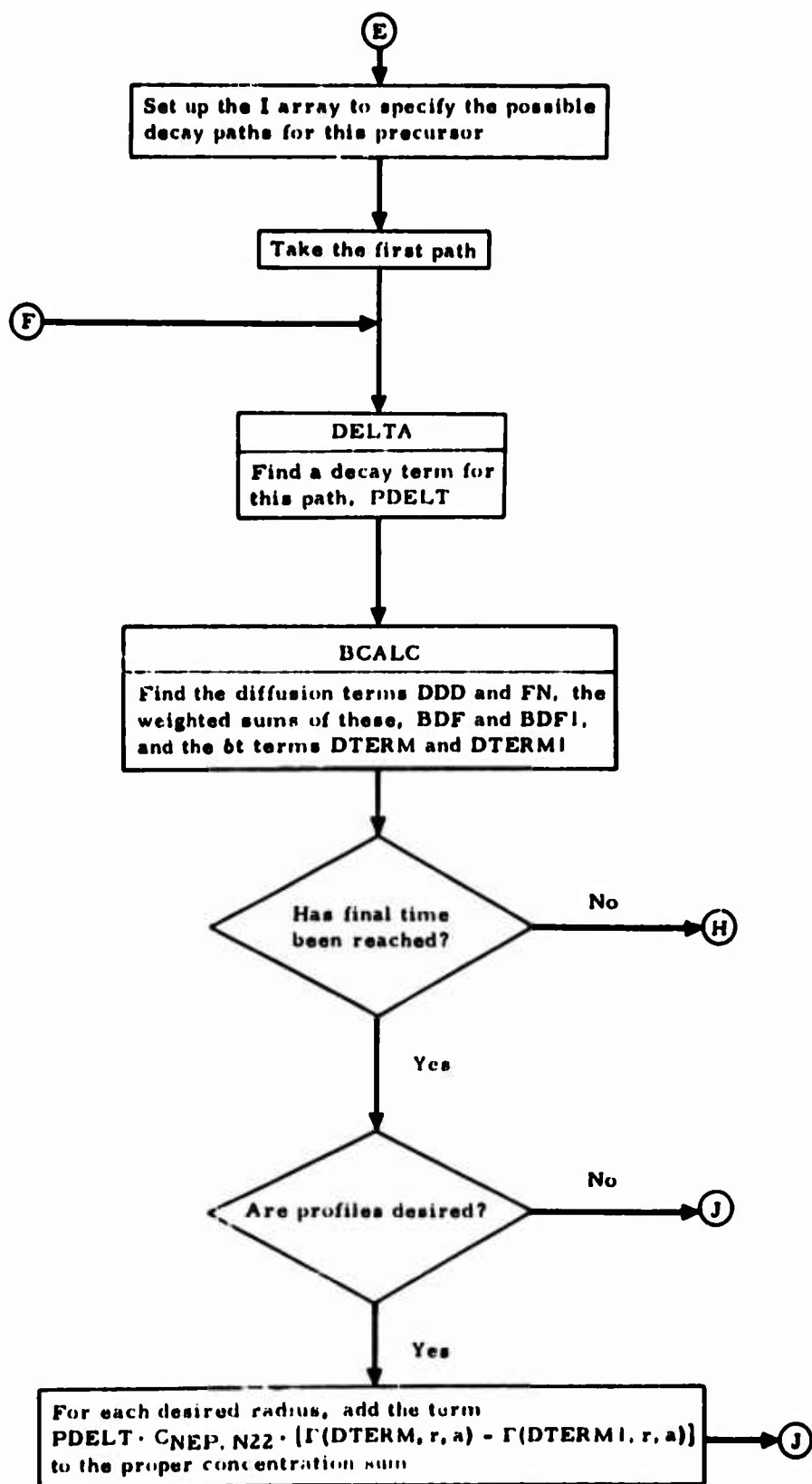


Fig. 2--Flow chart, main loop NORMAN (Sheet 3 of 5)

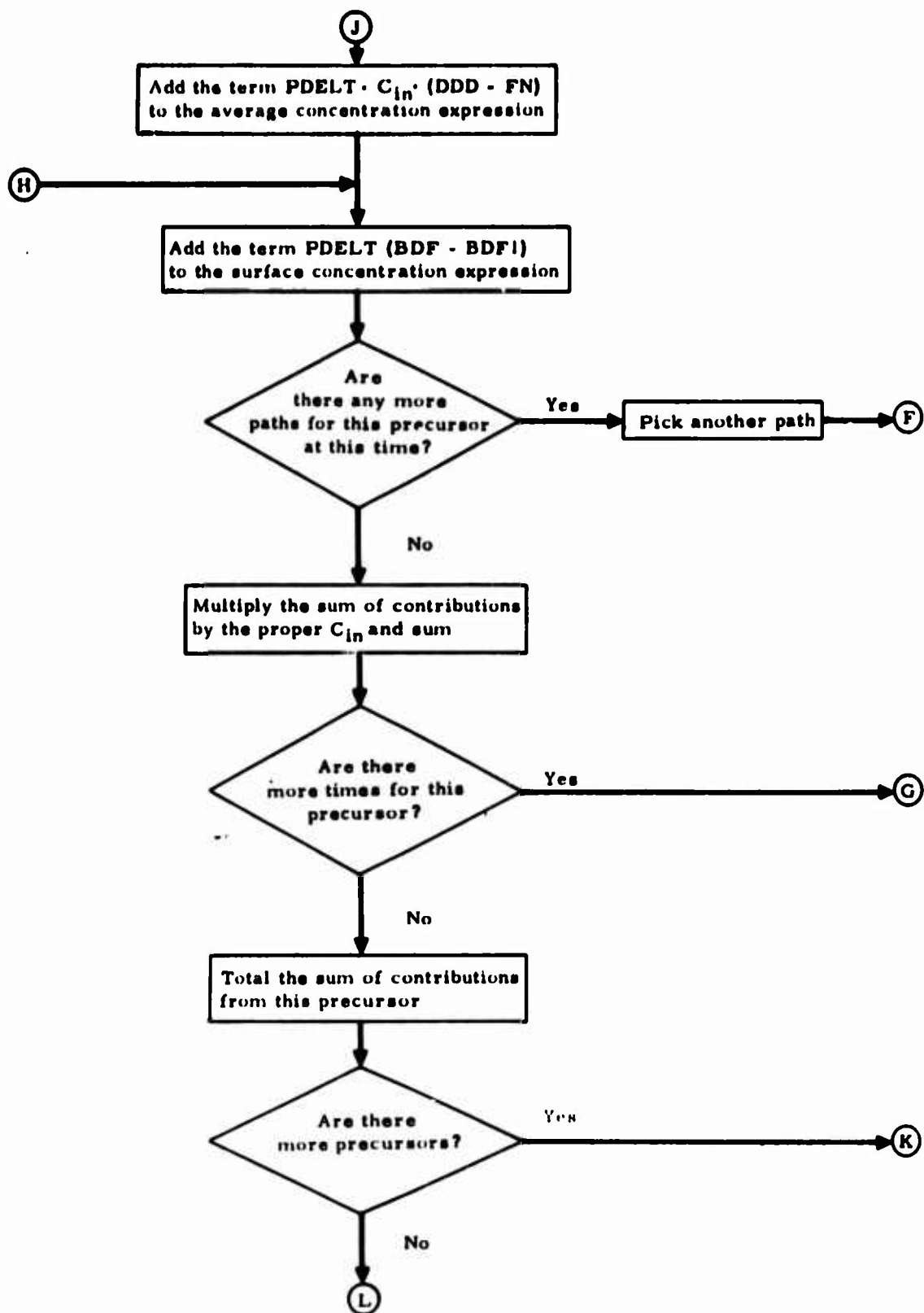


Fig. 2--Flow chart, main loop NORMAN (Sheet 4 of 5)

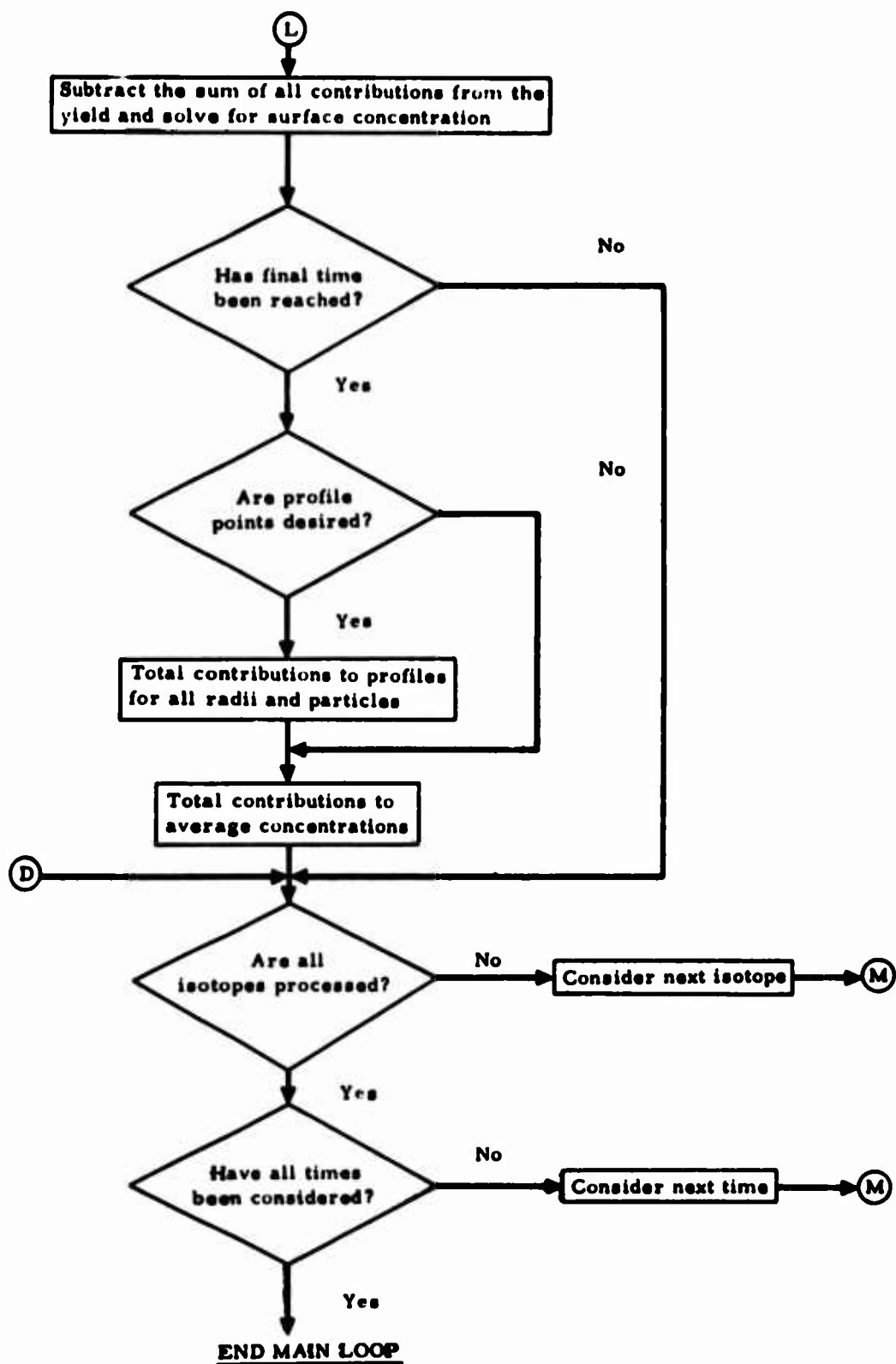


Fig. 2--Flow chart, main loop NORMAN (Sheet 5 of 5)

forming the product as in Eq. (5) and adding to the previous summed contributions. In the event that the final time step has been reached, add the appropriate terms to the average concentration and profile point sums.

3. Let α represent the total of the sum of all contributions to the average concentration expression except that term due to absorption diffusion of this isotope from surface concentration C_{in} . Then the surface concentration is found from

$$C_{in} \left(\frac{WMOL_i H_{in} V_n}{RT_n} + WN_{in} \right) = Y_{in} - \alpha$$

4. 2. 3. Output

Certain other calculations, as follows, are made while printing out results.

1. Calculation of the amount of material remaining in the gas phase for each isotope at each time:

$$GAS_{in} = \frac{C_{in} H_{in} V_n WMOL_i}{RT_n}$$

2. Computation of the amount of material in the solid phase (diffused), per isotope, at the final time:

$$SOLID_i = \sum_{s=1}^P A_{is} w_s$$

where A_{is} is the average concentration of isotope i in particle size s .

3. Computation of the weighted mean average concentration for each isotope i :

$$\bar{A}_i = \frac{SOLID_i}{(\text{total weight})}$$

The following quantities are printed:*

- a. T_n , t_n , and C_{in} for each i, n
- b. T_n , t_n , and GAS_{in} for each i, n
- c. T_N , r_s , and A_{is} , N being the final time and for each i, s
- d. \bar{A}_i for each i
- e.† $C_{is}(r)$ for each r, i, s , where $C_{is}(r)$ is the concentration of isotope i in particle s at radius r
- f. A summary of the amounts of material in gas and solid phases at the final temperature

4. 3. FUNCTION DIFFUS (DT, R)

This function computes a solution to the diffusion equation for a spherical body of radius r . The true solution is:⁽⁵⁾

$$D = 1 - \frac{6}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp(-n^2 \pi^2 \delta t / r^2) \quad (12)$$

or

$$D = 6 \left(\frac{\delta t}{r^2} \right)^{1/2} \left(\pi^{-1/2} + 2 \sum_{n=1}^{\infty} \text{ierfc} \frac{nr}{\sqrt{\delta t}} \right) - 3 \left(\frac{\delta t}{r^2} \right), \quad (13)$$

where⁽⁶⁾

$$\text{ierfc}(x) = \int_x^{\infty} \text{erfc}(u) du$$

and

$$\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-u^2} du.$$

* See Appendix D for sample output.

† This printout and the calculation are optional (see Section 2).
(See Appendix A for details.)

Function DIFFUS uses the following approximations to these solutions:

$$\text{Let } x = r/\sqrt{\delta t}$$

1. If $x > 3.14$,

$$D = \frac{3}{x} \left(\frac{2}{\sqrt{\pi}} - \frac{1}{x} \right) ,$$

which is a truncation of Eq. (13) with the infinite series neglected.

2. If $2.0 < x \leq 3.14$,

$$D = 1 - \frac{6}{\pi} \left[\exp(-\pi^2/x^2) + \frac{1}{4} \exp(-4\pi^2/x^2) \right]$$

3. If $0.745 < x \leq 2.0$,

$$D = 1 - \frac{6}{\pi} \left[\exp(-\pi^2/x^2) \right]$$

4. If $x \leq 0.745$,

$$D = 1 ,$$

where 2, 3, and 4 are truncations of Eq. (12).

The errors incurred by these approximations are bounded as follows:

$$\begin{aligned} |E_4| &\leq 2.5 \times 10^{-8} \\ |E_3| &\leq 1 \times 10^{-5} \\ |E_2| &\leq 1 \times 10^{-5} \\ |E_1| &\leq 5 \times 10^{-6} \end{aligned}$$

where E_i is the error using approximation i.

4. 4. SUBROUTINE FINAL (AVCON, GAS, R, WT, NAME)

Subroutine FINAL computes the concentration of the last isotope in the various particles assuming that

1. All other isotopes have completely decayed into the last one
2. None of the last isotope has decayed away

3. All of the material in the gas phase when the main process was terminated has condensed onto the particles according to surface area

Let a_{is} = average concentration of isotope i in particle of size s .

$Z_s = r_1 / r_s$, where r_1 is the radius of the largest particles, and

g_i = amount of isotope i in the gas phase when main process was terminated.

Then,

$$f_s = \sum_{i=1}^{LC} a_{is}$$

$$G = \sum_{i=1}^{LC} g_i$$

$$V_s = Z_s w_s \text{ (proportional to the surface area)}$$

$$v = \sum_{s=1}^P V_s$$

where w_s = weight of particles of size s .

Also,

$$F_s = \frac{Z_s G}{v} + f_s$$

and

$$W_s = F_s w_s ,$$

where F_s = total average concentration (includes gas condensation) in particle of size s

W_s = total weight of isotope in particle of size s

f_s = average concentration in particle of size s due to the decay of solids.

The average concentration of the last isotope of the chain, f_s , is considered to be equal to the sum of the average concentrations of all the members of the chain when the main process was terminated. Subroutine FINAL also lists out f , F , and W for each particle size.

4. 5. FUNCTION PROFIL (DT, r, Q)

Function PROFIL computes the concentration at a distance $a = rQ$ from the center of a spherical particle of radius r . The value of the concentration is found from the expression:⁽⁵⁾

$$\frac{C}{C_0} = 1 + \frac{2r}{\pi a} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin \frac{n\pi a}{r} e^{-n^2 \pi^2 \delta t / r^2} \quad (14)$$

or

$$\frac{C}{C_0} = \frac{r}{a} \sum_{n=0}^{\infty} \left\{ \operatorname{erfc} \left[\frac{(2n+1)r - a}{2\sqrt{\delta t}} \right] - \operatorname{erfc} \left[\frac{(2n+1)r + a}{2\sqrt{\delta t}} \right] \right\}, \quad (15)$$

where r = radius of particle

a = distance from center of particle, $a \geq 0.1r$

C_0 = surface concentration (assumed constant)

Function PROFIL computes the value of the ratio C/C_0 using a truncation of Eq. (14) or Eq. (15). In all cases, the series is terminated when either

$$\frac{|S_n - S_{n-1}|}{|S_n|} < \epsilon^*$$

or when $n > 100$, where S_k is Eq. (14) or Eq. (15) truncated to k terms.

The series used is chosen using the following criteria:

If $\delta \Delta t < b_j$, Eq. (15) is used where j is determined as the smallest integer such that

$$r \geq 10^{-j},$$

where $b_j = 10^{1-j - [(j-1)/2]}$

and where $[x]$ = greatest integer I such that $I \geq x$.

Otherwise Eq. (14) is used.

* $\epsilon = 0.01$ at present.

This scheme was determined by examining the values of Eqs. (14) and (15) for various numbers of terms and picking the equation that required the least number of terms.

4.6. FUNCTION ERF(X)

Function ERF computes an approximate value of the error function using a rational approximation. The error function is defined as:

$$\text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} dt .$$

ERF uses the approximation⁽⁵⁾

$$\text{erf}(x) = 1 - (a_1 t + a_2 t^2 + a_3 t^3) e^{-x^2}$$

where

$$t = \frac{1}{1 + px}$$

and

$$p = 0.47047$$

$$a_1 = 0.3480242$$

$$a_2 = -0.0958798$$

$$a_3 = 0.7478556$$

The error E in this approximation is bounded by

$$|E| \leq 2.5 \times 10^{-5} .$$

4.7. SUBROUTINE DELTA (N, NT, I, PR)

Subroutine DELTA computes the decay coefficient, PR, associated with decay of isotope i to the presently considered isotope at time NT. The array I specifies the path being taken, with I(1) specifying the time at which i is considered.

A product of terms of the form*

$$d_{inm} (1 - d_{i, m+1, m+1})$$

is found. The d array is initially calculated in the main routine in such a way that

$$d_{inm} = 1 \quad \text{if } n > m.$$

The general product then has the form

$$PR = d_{inm} (1 - d_{i, m+1, m+1}) d_{k, m+2, \ell} (1 - d_{k, \ell+1, \ell+1}) \cdots d_{n, r, NT-1}$$

where i is the subscript of the isotope presently under consideration. The values of n, ℓ , and r depend on the path.

4.8. SUBROUTINE BCALC (N, NT, I, KLAG, B, DD, DT)

This routine computes the correct δt term associated with the path specified by I and calls DIFFUS to solve for a diffusion term.

The δt term described by Eq. (A-10) is computed from the relation

$$\delta t = \sum_{p=n}^m \delta_{ip} \Delta t_p + \sum_{p=k}^{\ell} \delta_{(i+1)p} \Delta t_p + \cdots + \sum_{p=v}^q \delta_{(i+r)p} \Delta t_p,$$

where n, m, k, ℓ , \dots , v, and q are specified by the I array. The corresponding diffusion terms,

$$D_{i, n, m; i+1, k, \ell; \dots; i+r, v, q}^{(s)}$$

are then found by calling DIFFUS for each s. Depending upon KLAG, either the first D or the second D in Eq. (A-9) is found and stored in the DD array. δt is stored in DT and the expression

$$\sum_{s=1}^P (D_{i, n, m; i+1, k, \ell; \dots; i+r, v, q}^{(s)})^{w_s}$$

is stored in B.

* See Section 4.1, item 6 for definition of d_{inm} .

APPENDIX A
DERIVATION OF EQUATIONS USED

A. 1. THE GENERAL TERM IN THE SURFACE CONCENTRATION EQUATION

An analysis of the case of a single stable isotope with no precursors, which eliminates the decay question, makes it easier to understand the general case. If Eqs. (1) and (2) in Section 3 are rewritten leaving out the isotope identification and letting $w_1 = 1$ and $p = 1$, the following equations are obtained:

$$C_1 G_1 + C_1 D_{11} = Y \quad (A-1)$$

and

$$C_2 G_2 + C_1 D_{12} + (C_2 - C_1) D_{22} = Y, \quad (A-2)$$

where

$$G_N = \frac{V_N M H_N}{RT_N}.$$

Equation (A-2) can be rewritten as follows:

$$C_2 G_2 + C_2 D_{22} + C_1 (D_{12} - D_{22}) = Y.$$

The expression at t_3 is

$$C_3 G_3 + C_1 D_{13} + (C_2 - C_1) D_{23} + [C_3 - (C_2 - C_1) - C_1] D_{33} = Y$$

or

$$C_3 G_3 + C_1 D_{13} + (C_2 - C_1) D_{23} + (C_3 - C_2) D_{33} = Y.$$

The expression at t_4 is

$$C_4 G_4 + C_1 D_{14} + (C_2 - C_1) D_{24} + (C_3 - C_2) D_{34} + (C_4 - C_3) D_{44} = Y.$$

The expression at step N is then

$$C_N G_N + C_1 D_{1N} + \sum_{k=2}^N (C_k - C_{k-1}) D_{kN} = Y . \quad (A-3)$$

Equation (A-3) can be rewritten as follows:

$$C_N G_N + C_1 D_{1N} + \sum_{k=2}^N C_k D_{kN} - \sum_{k=1}^{N-1} C_k D_{k+1, N} = Y$$

or

$$C_N G_N + \sum_{k=1}^N C_k D_{kN} - \sum_{k=1}^{N-1} C_k D_{k+1, N} = Y$$

or, finally, as

$$C_N (G_N + D_{NN}) + \sum_{k=1}^{N-1} C_k (D_{kN} - D_{k+1, N}) = Y . \quad (A-4)$$

Next, consider the general expression with decay from precursors. Figure A.1 represents n isotopes at N time steps; the connecting lines represent the ways in which decay can occur. The numbers occurring with each state represent the number of ways in which that isotope at that time can decay to isotope 1 at t_N . It is apparent that if $N \leq n$, the diagram is triangular and is a Pascal's triangle, the numbers representing binomial coefficients. Thus for $N \leq n$, the total number of terms in the surface concentration expression is

$$2^0 + 2^1 + 2^2 + \dots + 2^{N-1} = 2^N - 1 .$$

For $N > n$, the diagram is a truncated Pascal's triangle. In this case, there are $2^n - 1$ terms from the purely triangular portion, plus

$$\sum_{k=0}^{n-1} \left[\sum_{j=n}^{N-1} \binom{j}{k} \right]$$

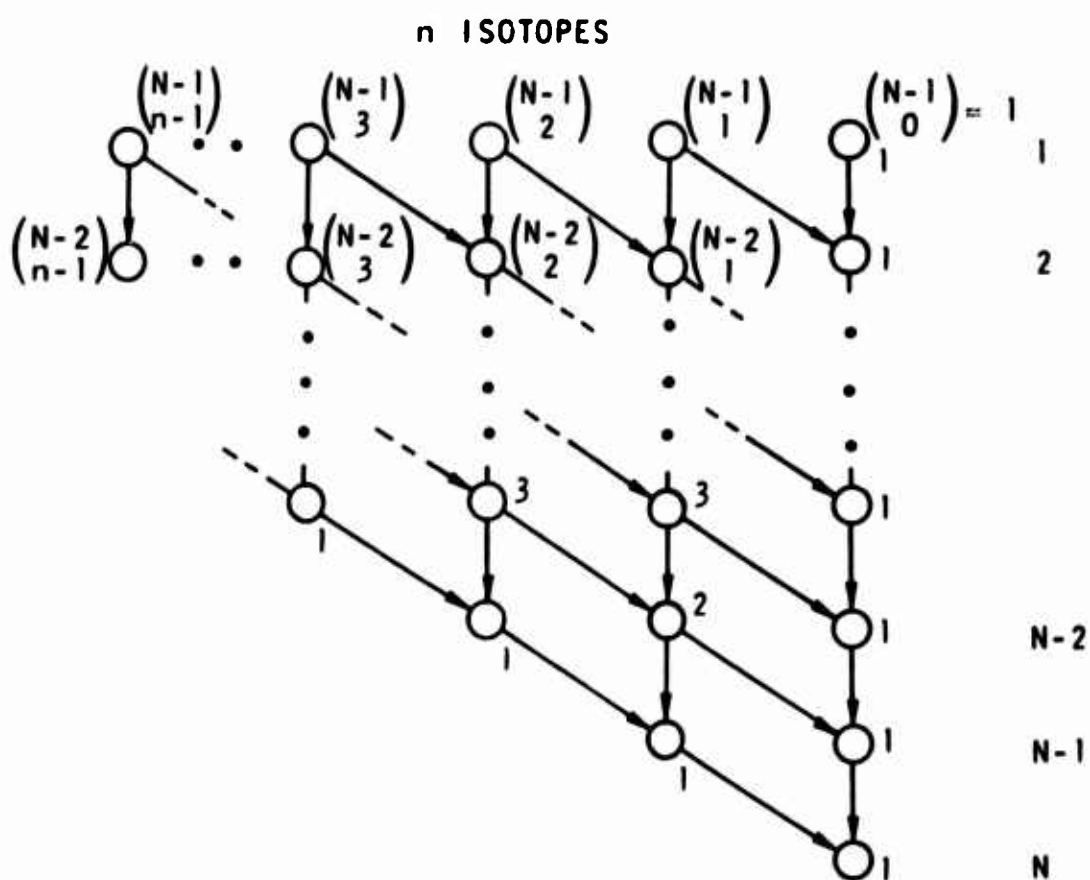


Fig. A. 1--Decay paths for n isotopes through N time steps

from the rectangular portion, giving a total of

$$M = \sum_{k=0}^{n-1} \left[\sum_{j=n}^{N-1} \binom{j}{k} \right] + 2^n - 1 \quad (\text{A-5})$$

In Eq. (A-4), each term in the sum consists of a surface concentration times a diffusion term. In each case the diffusion term is the difference of two diffusion terms, one representing diffusion from t_k to t_N and the other from $t_{(k+1)}$ to t_N . Each of the M terms in the general expression is of a similar form, modified by a decay term.

As an example, consider the terms associated with the position $n = 2$ in Fig. A.1 at t_4 . There are three possible paths for decay to isotope 1. The decay coefficients associated with these paths are

$$\left. \begin{aligned} (1 - d_{211})d_{123} \\ d_{211}(1 - d_{222})d_{133} \\ d_{212}(1 - d_{233}) \end{aligned} \right\} \quad (\text{A-6})$$

where d_{inm}^* represents the decay coefficient of isotope i from time step Δt_n through Δt_m . The corresponding isotope indexed diffusion terms are:

$$\left. \begin{aligned} D_{2,1,1;1,2,4} - D_{1,2,4} \\ D_{2,1,2;1,3,4} - D_{2,2,2;1,3,4} \\ D_{2,1,3;1,4,4} - D_{2,2,3;1,4,4} \end{aligned} \right\} \quad (\text{A-7})$$

where $D_{i,n,m;i+1,k,\ell;\dots;i+r,v,q}$ represents diffusion as isotope i from t_n to t_m , as isotope $i+1$ from t_k to t_ℓ , etc., and as isotope $i+r$ from time t_v to t_q^\dagger (see Eq. (A-10)).

* See Section 4.1, item 6.

† Note that decay is carried only through Step 3, while diffusion is carried through Step 4 (see Section 3).

The total contribution to isotope 1 at t_4 from isotope 2 at t_1 can be written as

$$\begin{aligned}
 C_{21} [(1 - d_{211})d_{123}(D_{2,1,1;1,2,4} - D_{1,2,4}) \\
 + d_{211}(1 - d_{222})d_{133}(D_{2,1,2;1,3,4} - D_{2,2,2;1,3,4}) \\
 + d_{212}(1 - d_{233})(D_{2,1,3;1,4,4} - D_{2,2,3;1,4,4})] \quad (A-8)
 \end{aligned}$$

where again a single particle of unit weight is assumed.

From the above discussion it can be seen that the general term is of the form

$$\begin{aligned}
 C_{in} d_{inm} (1 - d_{i,m+1,m+1}) d_{i+1,m+2,k} (1 - d_{i+1,k+1,k+1}) \cdots \\
 \cdots d_{i+r,\ell,N-1} \left[\sum_{s=1}^P (D_{i,n,m+1;i+1,m+2,k+1;\cdots;i+r,\ell,N}^{(s)} \right. \\
 \left. - D_{i,n+1,m+1;i+1,m+2,k+1;\cdots;i+r,\ell,N}^{(s)} w_s \right] \quad (A-9)
 \end{aligned}$$

where

1. We are considering the contribution to isotope $i + r$ at time N via some path, from isotope i at time n .
2. $m \geq n + 1$
 $k \geq m + 1$
 \vdots
 $\ell \geq i + r$
3. There are p particle sizes with weights w_1, w_2, \dots, w_p .
4. If $n > m$, $d_{inm} = 1$ as a mathematical convenience.

The quantity $D_{i,n,m;i+1,k,\ell;\cdots;i+r,v,q}^{(s)}$ represents a solution of the diffusion equation for a particle of radius r_s and δt term given by

$$\delta t = \sum_{n=q}^n \delta_{in} \Delta t_n + \sum_{n=k}^{\ell} \delta_{i+1,n} \Delta t_n + \cdots + \sum_{n=v}^q \delta_{i+r,n} \Delta t_n \quad (A-10)$$

where δ_{in} is defined by Eq. (11), Section 4.1, item 8, and Δt_n is defined by Eq. 7, Section 4.1, item 4.

A. 2. AVERAGE CONCENTRATIONS AND PROFILES

As in the case of surface concentrations, the case considered is that of a single stable isotope with no precursors. The basic relationship is

$$\frac{\bar{C}}{C} = D, \quad (A-11)$$

where \bar{C} is an average concentration increment, C is a surface concentration increment, and D is a diffusion term as in Section A. 1. At the first time step, it is clear that

$$\bar{C}_1 = C_1 D_{11}.$$

At the second time step,

$$\bar{C}_2 = C_1 D_{12} + (C_2 - C_1) D_{22},$$

where the first term on the right represents the concentration at time step 1 further diffused and the second term represents material condensed and diffused during time step 2. Similarly, at time step 3,

$$\bar{C}_3 = C_1 D_{13} + (C_2 - C_1) D_{23} + (C_3 - C_2) D_{33},$$

where the three terms represent, respectively, condensation during time steps 1, 2, and 3, and diffusion from those times to time 3. At time step N , it follows that

$$\bar{C}_N = C_1 D_{1N} + \sum_{k=2}^N (C_k - C_{k-1}) D_{k,N}, \quad (A-12)$$

where each term in the sum represents a concentration diffused over the specified time interval.

To obtain an expression similar to Eq. (A-4), Eq. (A-12) is rewritten

as

$$\bar{C}_N = C_1 D_{1N} + (C_N - C_{N-1}) D_{N,N} + \sum_{k=2}^{N-1} C_k D_{k,N} - \sum_{k=2}^{N-1} C_{k-1} D_{k,N} ,$$

or

$$\bar{C}_N = C_N D_{N,N} + \sum_{k=1}^{N-1} C_k D_{k,N} - \sum_{k=1}^{N-1} C_k D_{k+1,N} ,$$

or, finally, as

$$\bar{C}_N = C_N D_{N,N} + \sum_{k=1}^{N-1} C_k (D_{k,N} - D_{k+1,N}) . \quad (A-13)$$

It can be seen that the general expression including decay from precursors consists of terms similar to Eq. (A-9). The number of such terms is the same as that described in Section A.1, since there is a contribution from each isotope at each preceding time step for each possible decay path. Here the expression for average concentration in the s^{th} particle size consists of terms of the form:

$$\begin{aligned} & C_{in} d_{inm} (1 - d_{i,m+1,m+1}) d_{i+1,m+2,k} (1 - d_{i+1,k+1,k+1}) \cdots \\ & \cdots d_{i+r,\ell,N-1} D_{i,n,m+1;i+1,n+2,k+1;\cdots;i+r,\ell,N}^{(s)} \\ & - D_{i,n+1,m+1;i+1,m+2,k+1;\cdots;i+r,\ell,N}^{(s)} \end{aligned} \quad (A-14)$$

summed over all contributions.

To find profiles, it is desired to find the concentration at specific points within the particle. The basic relation here is (see Ref. 6)

$$\frac{C(a)}{C} = \Gamma(a, r, \delta t) , \quad (A-15)$$

$$\text{where } \Gamma(a, r, \delta t) = 1 + \frac{2r}{\pi a} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \sin \frac{n\pi a}{r} \exp(-n^2 \pi^2 \delta t / r^2) .$$

As with average concentrations, Eq. (A-15) gives a concentration increment due to diffusion during the given time and with zero initial concentration. For a stable isotope with no precursors we can, in an analagous manner, obtain the expression

$$C_{iN}(a) = C_{iN} \Gamma(a, r, \delta_{iN} \Delta t_N) + \sum_{k=1}^{N-1} C_{ik} \left[\Gamma\left(a, r, \sum_{n=k}^N \delta_{in} \Delta t_n\right) - \Gamma\left(a, r, \sum_{n=k+1}^N \delta_{in} \Delta t_n\right) \right] \quad (A-16)$$

and in the general case obtain a sum of terms similar to Eq. (A.14) with each D replaced by the appropriate Γ .

APPENDIX B

MODEL CALCULATIONS

Some of the initial results of calculations obtained using this program are considered in this appendix. In these calculations examples of a refractory and a volatile chain, 95 and 137, respectively, were selected for study. The results should demonstrate the difference in behavior for extreme cases of refractory and volatile nuclide chains with varying conditions and thus provide limits of fission product behavior during fallout formation. Data sources for these calculations have been listed earlier. In addition to these sources, the standard particle distribution shown in Table B. 1 was developed from one used by Miller, * experimental and estimated diffusion coefficients were employed as measured or estimated in reported studies, and total fissions were scaled as a function of weapon fission yield according to Miller. ⁽¹⁾

Several program variables had to be investigated in order to demonstrate the degree of dependence of the calculational system on these variables. For instance, the variation of results with the size of the temperature increment must be vanishingly small for the selected temperature increment as smaller increments are considered. Also, the variation of results with choice of initial and final calculational temperatures should be defined. Finally, the fact that the particle size distribution employed is idealized—that is, some selected radii represent all of the mass of the particles—should be considered. These points have been investigated and seem to be satisfactorily understood as will be demonstrated as the calculations are presented.

The calculations for the 95 and 137 chains (neglecting $I^{137} \rightarrow Xe^{136}$ and $I^{138} \rightarrow Xe^{137}$) were performed using 2700°K as an initial temperature, 200°K increments, terminating at 900°K, and employing the particle distribution described in Table B. 1. The size of the detonation was taken as 100 KT pure fission. The amount of soil associated with the cloud was 8.5×10^9 g.

* Miller, C. F., private communication, November 1965.

Table B. 1
STANDARD PARTICLE SIZE DISTRIBUTION

Designation	Particle Radius (cm)	Weight Percent of Particle Fraction
T	0. 00030	0. 38
S	0. 0030	28. 92
M	0. 0154	60. 2
L	0. 13	10. 5

The calculated descriptions of behavior of the 137 and 95 chains are presented in Figs. B. 1 and B. 2, respectively. In these figures, the average concentration of a particular nuclide in the chain is presented as a function of the last temperature for which the adsorption-diffusion process was calculated. Also included are the gas phase contents of the nuclides at the same temperatures (designated by open circles). In the phenomena described in Fig. B. 1, the curve for the tellurium gas phase content is decreasing as the result of two processes:

1. Te^{137} decay.
2. Absorption of Te^{137} in the fallout particles.

Corresponding processes are involved to different degrees in the description of the gas phase content of any nuclide. In the case of Te^{137} at the lowest temperature, so little of the Te^{137} has been absorbed that the gas phase content curve closely represents the tellurium decay. The gas phase content curves for iodine and xenon also essentially represent radioactive decay phenomena alone, since both of these elements are very volatile. On the other hand, the gas phase content of cesium is dropping sharply with temperature, not because Cs^{137} is decaying but, in this case, because 94% of the cesium in the system has been absorbed by the fallout particles by the 1900°K point and more is absorbed at lower temperatures. Thus, the cesium curve describes mainly the absorption process.

The average concentrations of Te^{137} as they vary with temperature and particle size were also investigated. The large particles, L, as defined in Table B. 1, show a slow but continuous increase in average tellurium concentration as the temperature decreases (see Fig. B. 1).

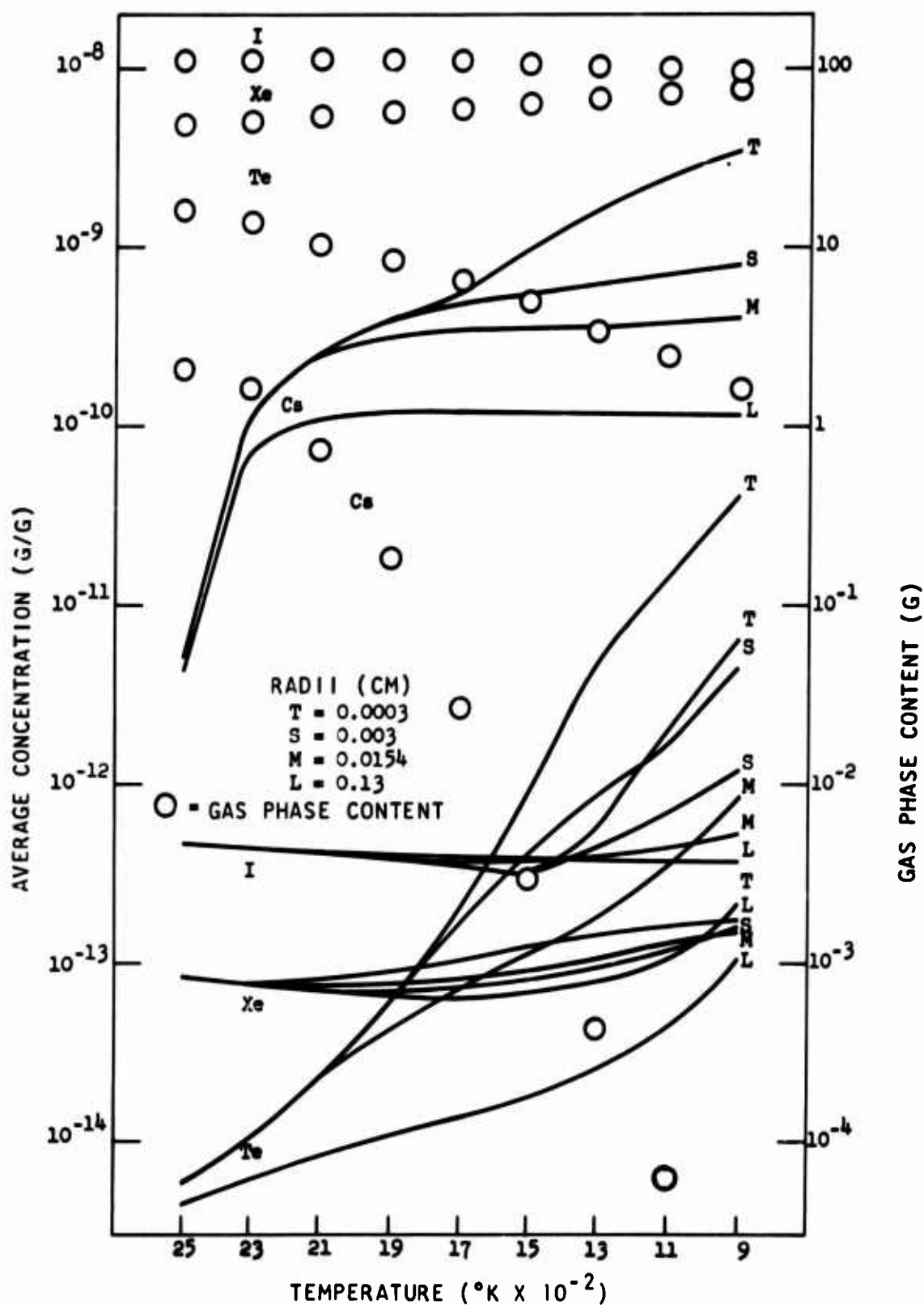


Fig. B. 1--Calculated absorption in fallout of members of 137 chain in g fission product per g fallout as a function of temperature and particle size

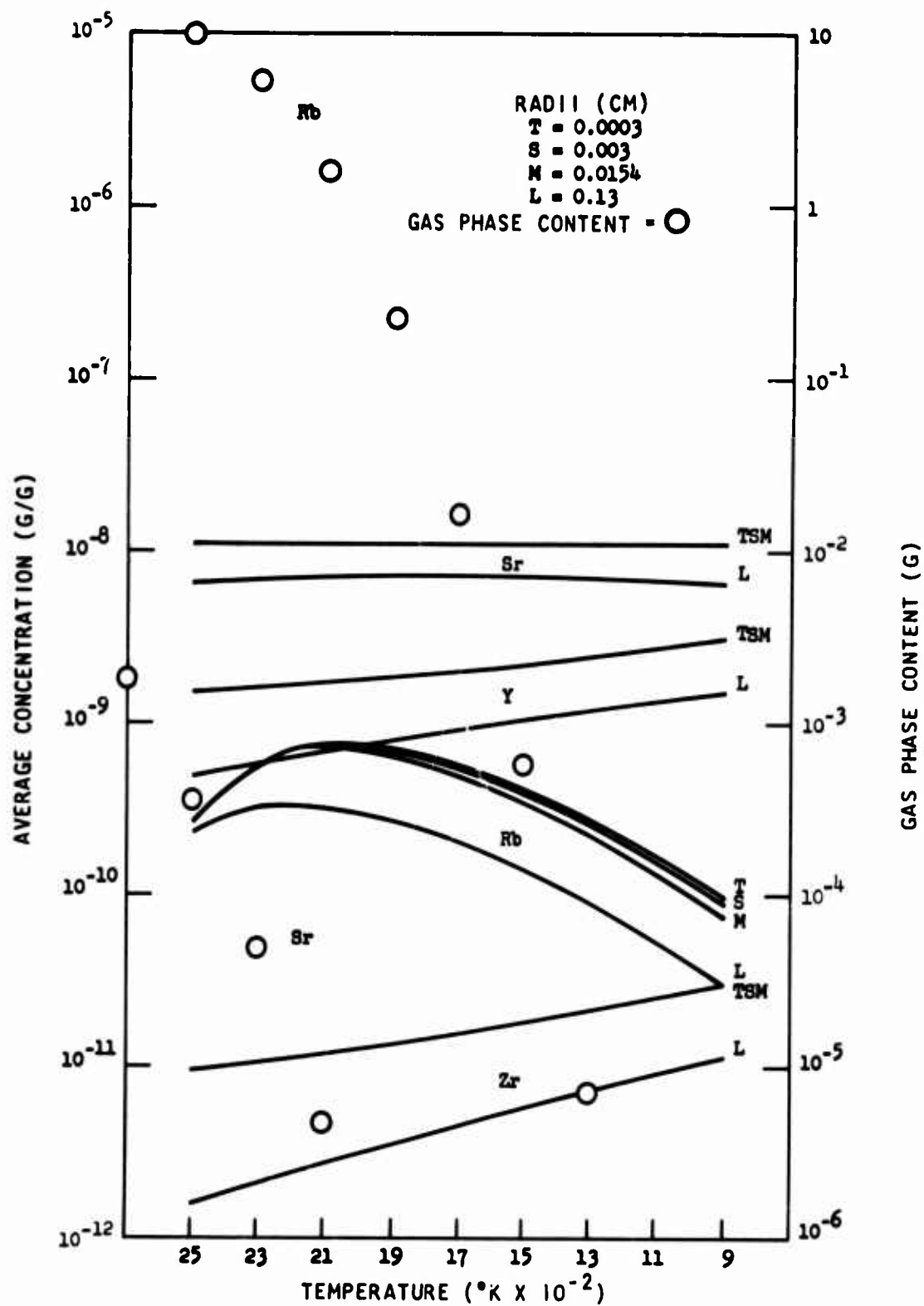


Fig. B.2--Calculated absorption in fallout of members of 95 chain in g fission product per g fallout as a function of temperature and particle size

Also, at the initial temperature the L particles exhibit a slightly lower concentration than the medium-sized particles, M. This point is important because it suggests that at the highest temperature of the calculation, the L particles did not equilibrate with the gas phase; that is, diffusion was not complete. In contrast, the tiny particles, T, the small particles, S, and the M particles exhibit essentially the same average concentration at the initial temperature. Further consideration of Fig. B.1 reveals that the L particles experience a somewhat smaller increase in tellurium concentration than the M particles as the temperature decreases. Also, the S and M curves exhibit a departure from the more sharply rising T curve at two different lower temperatures. Departure points from the T curve occur as the central portions of the L, S, and M particles effectively lose contact with the surface and diffusive transport begins to control the rate of absorption. In addition, at 1300°K absorption into the T particles is diffusion-controlled (at this temperature the surface concentration is calculated to be twice the average concentration).

The behavior of other elements in the 137 chain can also be observed in Fig. B.1. Neither iodine nor xenon is strongly absorbed at even the lowest temperature of this study. The higher temperature portions of the iodine and xenon curves in Fig. B.1 reflect the low absorption and a low temperature coefficient of absorption for these isotopes. At lower temperatures, however, the iodine curves reflect the behavior of the parent tellurium curves. That is, at these temperatures the main iodine concentration in the particles comes from absorbed tellurium decay to iodine, whose loss from the particle is diffusion-controlled. The low temperature increase in xenon concentration in the particles is due to iodine decay, and xenon loss is also diffusion-controlled. This latter process has just become apparent as a result of the lowest temperature calculations shown in Fig. B.1. Similar phenomena can be observed in the cesium absorption curves. Fission cesium is mainly absorbed at 2100°K , where the absorption curves in Fig. B.1 stop their steep ascent. This is the same

temperature region where gas phase cesium starts its sharp decrease. Note that the concentration of cesium in the L particles does not appreciably change at lower temperatures. The remaining gaseous cesium, and that formed in the gas phase decay of xenon, is picked up mainly by the smaller particles because of their large surface to volume ratio. The cesium concentration of the M particles does not change much after 1900°K , while that of the S particles begins to level off at 1700°K . The cesium concentration of the T particles increases sharply, reflecting the continued absorption of cesium produced from xenon (g).

The behavior of the 137 nuclide chain can thus best be explained in terms of diffusion-controlled sorption of tellurium and cesium and decay of the nuclides. Note that the sorption processes depicted in Fig. B.1 account for only a minor portion of the total mass of fission products of this nuclide chain. The rest of the material, at times subsequent to those of this calculation, will go through the process of decaying to cesium and depositing on the outer portions of the fallout particles or on any condensed phase with which it comes in contact. In this study, however, it is assumed that the material remaining in the gas phase at 900°K is surface-deposited on the fallout particles themselves, according to their surface area. In reality, xenon, with a relatively long half life (234 sec), may well separate from portions of the fallout particles before decaying and depositing.

Figure B.2 shows similar data for the 95 chain. The behavior depicted in this figure, except for that of rubidium, represents essentially complete absorption at the highest temperature of the study, 2700°K , and rubidium absorption is essentially complete by 1900°K . The absorption differences between the smaller particles and the L particles result from the nuclides in this chain being incompletely diffused in the larger particles at 2700°K . The splitting of the M, S, and T curves of rubidium results from diffusion control becoming important at lower temperatures for smaller particles, as was discussed previously for tellurium in the 137 chain.

A further description of the effect of initial temperature is appropriate here. Table B.2 contains the 900°K average concentration ratios of L and M for zirconium, yttrium, and strontium and the L/M, M/S, and S/T average concentration ratios for rubidium. For a highly absorbed species, the ratio L/M differs from unity but obviously will approach unity as starting temperatures are increased. However, for rubidium, which is not so highly absorbed, the concentration ratios in various sized particles are independent of the starting temperature; and the smaller the particles, the more nearly this value approaches unity. The calculational values for less highly absorbed species thus appear to be independent of starting temperature.

Table B. 2
CONCENTRATION RATIOS AT 900°K OF PARTICLES OF DIFFERENT
SIZE FOR VARIOUS STARTING TEMPERATURES

Starting Temperature (°K)	Average Concentration Ratio					
	Zr (L/M)	Y (L/M)	Sr (L/M)	Rb (L/M)	Rb (M/S)	Rb (S/T)
2700	0.378	0.497	0.611	0.398	0.844	0.950
3100	0.600	0.754	0.859	0.398	0.844	0.950
3900	0.862	0.924	0.883	0.398	0.844	0.950

The phenomenon of lack of equilibration of nonfractionated nuclides in the larger particles at high temperatures which is seen when the present model is used would seem to indicate some fractionation with size. An investigation of fallout should reveal whether this is indeed the case.

The orientation calculation described above has demonstrated many of the features of the diffusion-controlled model. These features seem to find some support in studies of fallout and certainly should be studied more thoroughly. However, before further questions concerning calculations of fallout phenomena are investigated, some of the strictly mathematical variations within the model calculations should be considered.

An investigation of different-sized temperature stepping intervals was made. In general, in the calculations reported here, 200°K temperature intervals were used. However, these test calculations, which were initiated at 2700°K and were carried through 900°K, were made for the two nuclide chains in both 200° and 100°K increments. Comparing results was more complicated than it first appeared because the final diffusion time corresponded to 800°K in the 200° interval calculations and to 850°K in the 100° interval calculations. In order to avoid this difficulty, both systems were allowed to decay and to absorb the resulting gaseous fission products (mainly Cs¹³⁷) according to surface area, thereby nearly eliminating the final calculational temperature differences. The comparison of results is presented in Table B.3. The only difference that seems significant occurred in the L particle zirconium concentrations, and it can apparently be explained by the difference in initial starting temperatures. The particles had essentially twice the time to diffuse at 2700°K in the case of the 200° increments as in the case of the 100° increments. While a better example might be constructed, it would appear from this study that the size of the temperature increment used in the model may not be very important if chosen as 200°K or less.

Table B. 3
EFFECT OF SIZE OF TEMPERATURE INCREMENT ON
FISSION PRODUCT ABSORPTION

Nuclide	Particle Size	Absorption (g)	
		100°C Temp. Interval	200°C (Std) Temp. Interval
Zr	T	0.456	0.456
	S	34.67	34.63
	M	71.52	71.17
	L	6.86	7.26
Cs	T	14.62	14.63
	S	112.40	112.44
	M	46.92	46.88
	L	1.045	1.042

In the investigation of the effect of the particle size distribution, three different distributions were studied under the same conditions. The distributions employed and the weights of soil associated with each distribution in this case are presented in Table B.4. The amounts of cesium and zirconium fission products (in grams) after decay of precursor fission products are also presented for each fallout particle size as in the previous case. Finally, a ratio of the cesium and zirconium average concentrations associated with each particle size is presented. This ratio is proportional to a fractionation factor ratio comparing these elements. The proportionality constant is 0.649, a nuclide chain yield ratio. Further consideration of Table B.4 reveals that fractionation factors for the very smallest particles far exceed unity, while for the larger particles these factors are less than unity. Fractionation factors in this model are thus quantities that depend on particle size (and also probably on the degree of detachment of the fallout particles from the nuclear cloud before conversion of volatile fission products to condensable ones). Therefore, if this model is correct, observed fractionation factors should be dependent on particle size and thus not accurately definable without ample description of this parameter. Indeed, these factors should be sensitive not only to the particle size in question but also to the particle size distribution. Specifically, one observes using distributions (2) and (3) that fractionation factors for the same size particles can differ considerably. Particle distribution (3) contains a large amount of very small particles. Distributions (1) and (2) are similar, since they both are based on Miller's description. * Note that the distributions (1) and (2) produce similar fractionation factors for similarly sized particles. It seems apparent that in testing this model for reproduction of fractionation factors, one must specify the particle size distribution, a factor often not well documented.

A study was made of the effect of the size of the detonation and the amount of soil in the cloud (that is, the proximity of the detonation to the

* Miller, C. F., private communication, November 1965.

Table B. 4
EFFECT OF PARTICLE SIZE DISTRIBUTION ON FISSION PRODUCT ABSORPTION

Particle Radius (cm)	Fallout (g)			Fission Product (g)						Ratio		
	Weight (1) (Std)	Weight (2)	Weight (3)	Cs (1)	Cs (2)	Cs (3)	Zr (1)	Zr (2)	Zr (3)	Cs/Zr (1) ²	Cs/Zr (2) ²	Cs/Zr (3) ²
10 ⁻⁶			8.5×10 ⁴			104.6			1.20			87.0
10 ⁻⁵		8.5	4.25×10 ⁵		0.078	52.7		1.17×10 ⁻⁴	6.01		667.0	8.8
10 ⁻⁴		5.95×10 ³	8.5×10 ⁵		5.50	11.0		0.0816	12.02		67.0	0.92
3×10 ⁻⁴	3.23×10 ⁴			14.6			0.444			33.0		
10 ⁻³		1.19×10 ⁶	2.975×10 ⁶		110.7	5.13		16.32	42.06		6.8	0.12
3×10 ⁻³	2.458×10 ⁶			112.4			33.73			3.3		
10 ⁻²		5.95×10 ⁶	2.89×10 ⁶		57.3	1.40		80.9	40.61		0.71	0.034
1.54×10 ⁻²	5.117×10 ⁶			46.9			69.28			0.68		
0.1		1.353×10 ⁶	8.5×10 ⁵		1.45	0.132		16.2	10.54		0.090	0.0125
0.13	8.725×10 ⁵			1.04			10.06			0.10		
1.0		8.415×10 ²	4.25×10 ⁵		9.6×10 ⁻⁵	9.8×10 ⁻³		2.05×10 ⁻³	1.07		0.046	0.0092

²Can be converted to fractionation factors by multiplying by 0.649.

land surface). The calculated final amounts of cesium and zirconium for the various particle sizes as a function of these two quantities are shown in Table B. 5. Note that the calculated fission product distributions in the particles were only slightly different for the various conditions. Specific activities per gram of fallout vary directly with yield and indirectly with the amount of soil, but the relative fission product distribution among the different-sized particles is not greatly affected by these parameters. This reemphasizes the importance of particle size distributions and chemistry in determining the fate of fission products during fallout formation.

Table B. 5

VARIATION OF FISSION PRODUCT ABSORPTION WITH SIZE
AND HEIGHT OF DETONATION EFFECTS FOR A
100-KT FISSION YIELD DETONATION

Particle Radius (cm)	Cesium Absorbed (g)			Zirconium Absorbed (g)		
	Standard	1/100 Soil	10 MT, Total Yield	Standard	1/100 Soil	10 MT, Total Yield
0.0003	14.63	14.76	13.84	0.444	0.539	0.432
0.003	112.44	113.20	110.21	33.73	35.54	32.86
0.0154	46.88	46.06	49.55	69.28	67.76	68.41
0.130	1.042	0.954	1.387	10.06	9.67	11.81

The computer program can also provide fission product profiles. Calculated profiles for both the 137 and 95 chains have been investigated for a 100-KT fission detonation, using 200° temperature increments and the particle size distribution given in Table B. 1. The calculations were initiated at 2700°K for the 137 chain and at 3100°K for the 95 chain. The 900°K profiles for the 95 chain are presented as a function of particle size in Fig. B. 3, and those for the 137 chain are presented in Figs. B. 4, B. 5, and B.6. An unusual abscissa scale is used in these figures solely for the purpose of demonstrating the calculated values more efficiently.

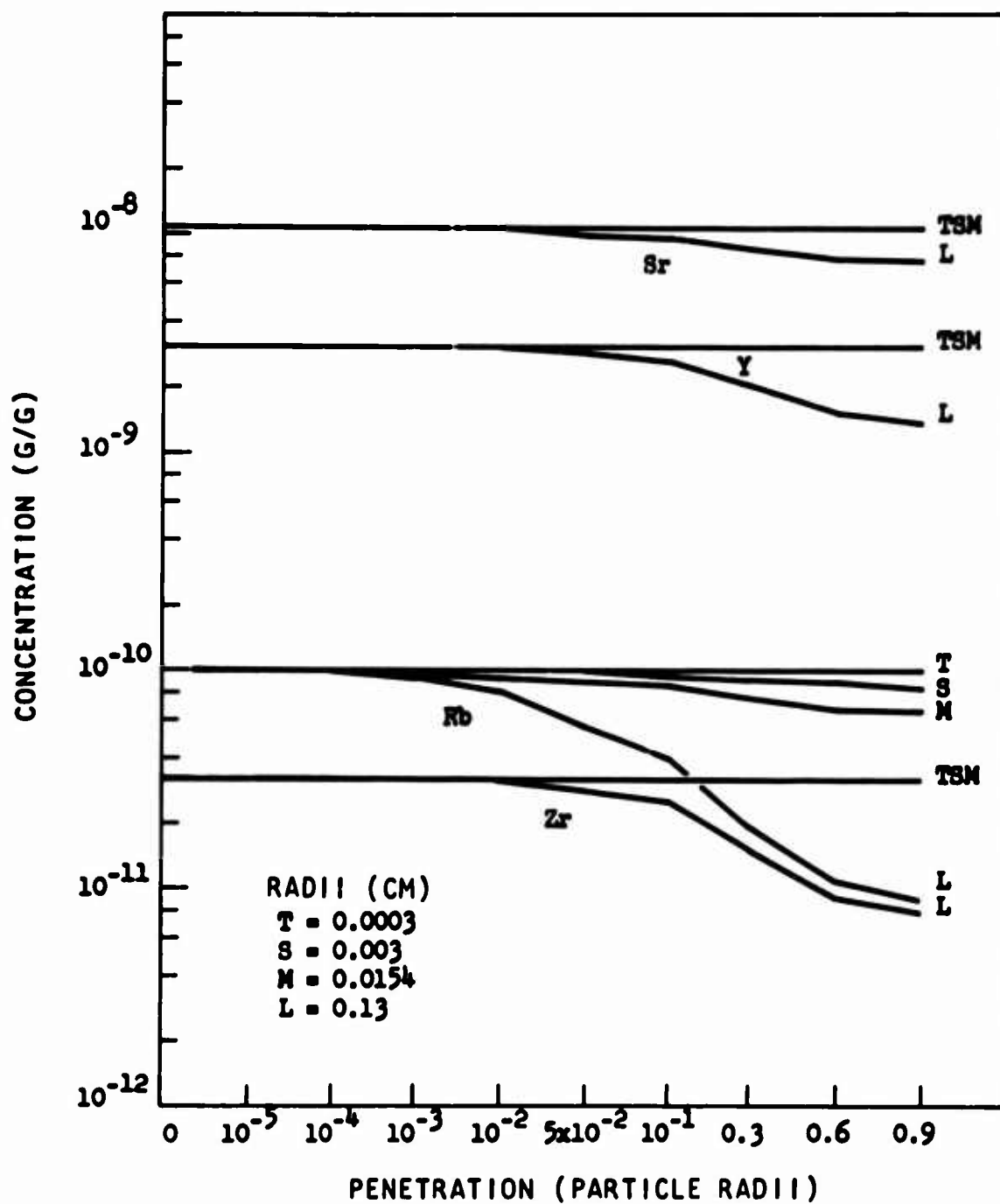


Fig. B. 3--Concentration profiles at 900°K of 95 nuclide chain members as a function of particle size for standard detonation

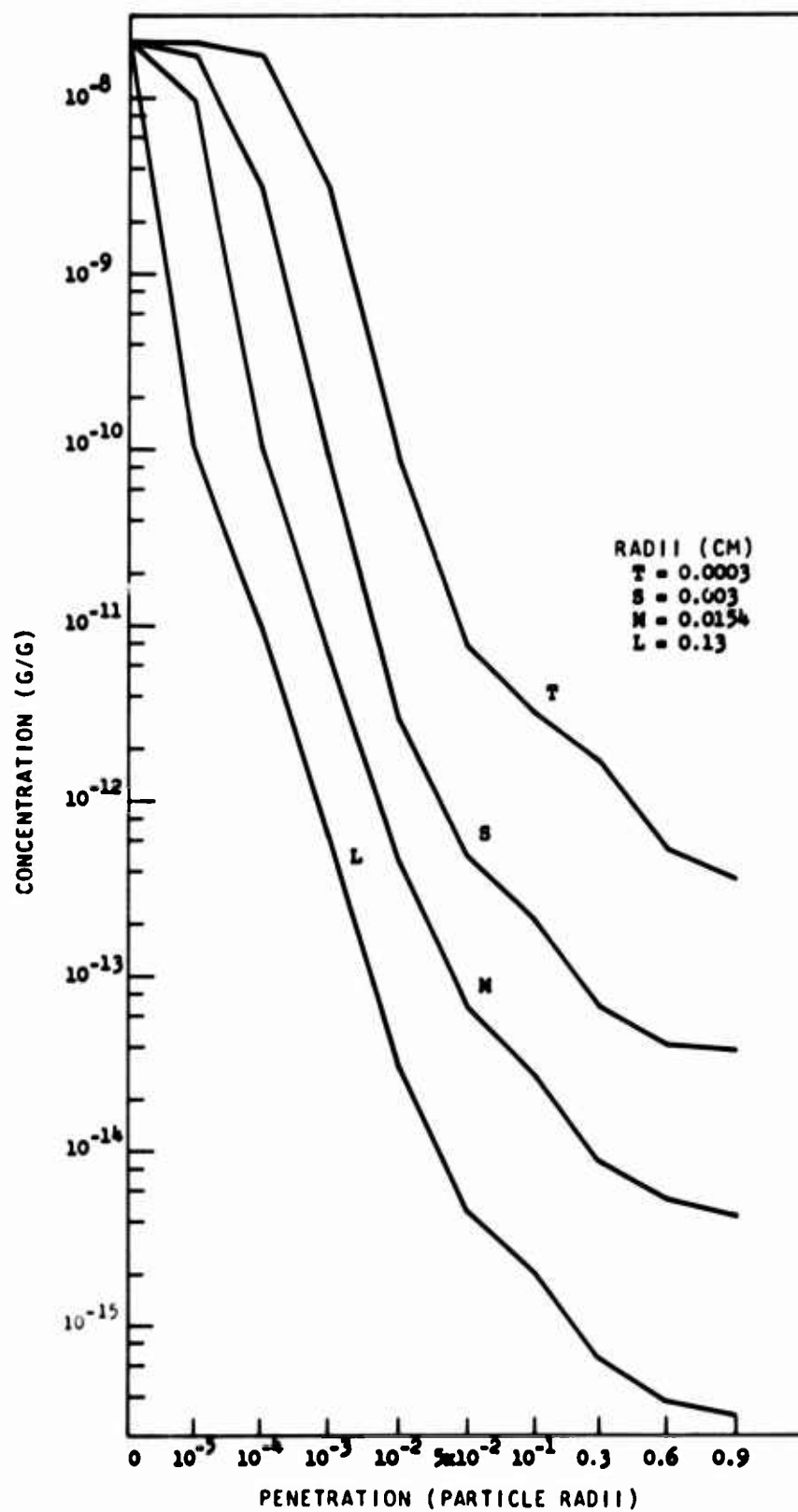


Fig. B. 4--Tellurium-137 concentration profiles at 900°K for standard particle size distribution and standard detonation

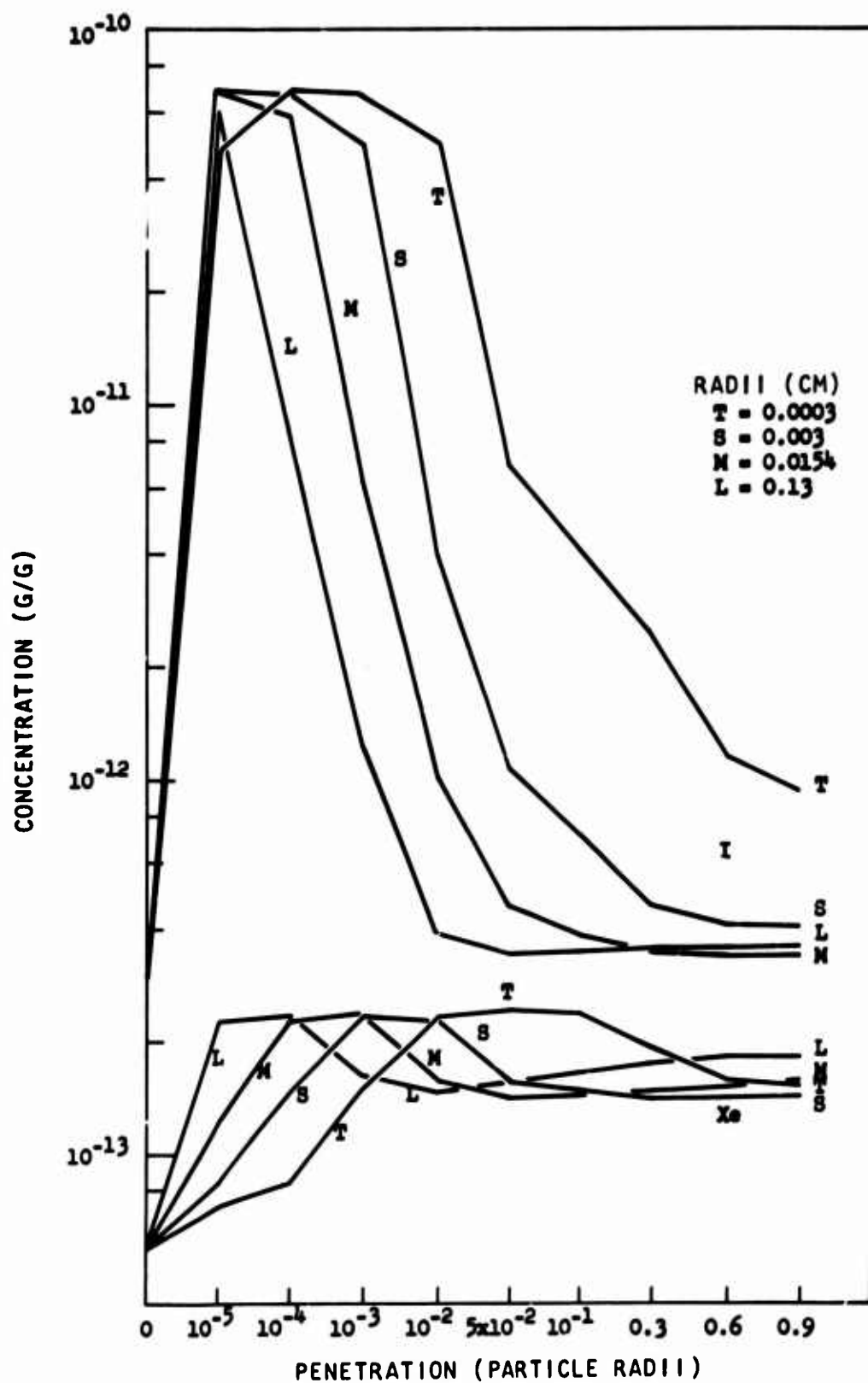


Fig. B. 5--Iodine and xenon-137 concentration profiles at 900°K for standard particle size distribution and standard detonation

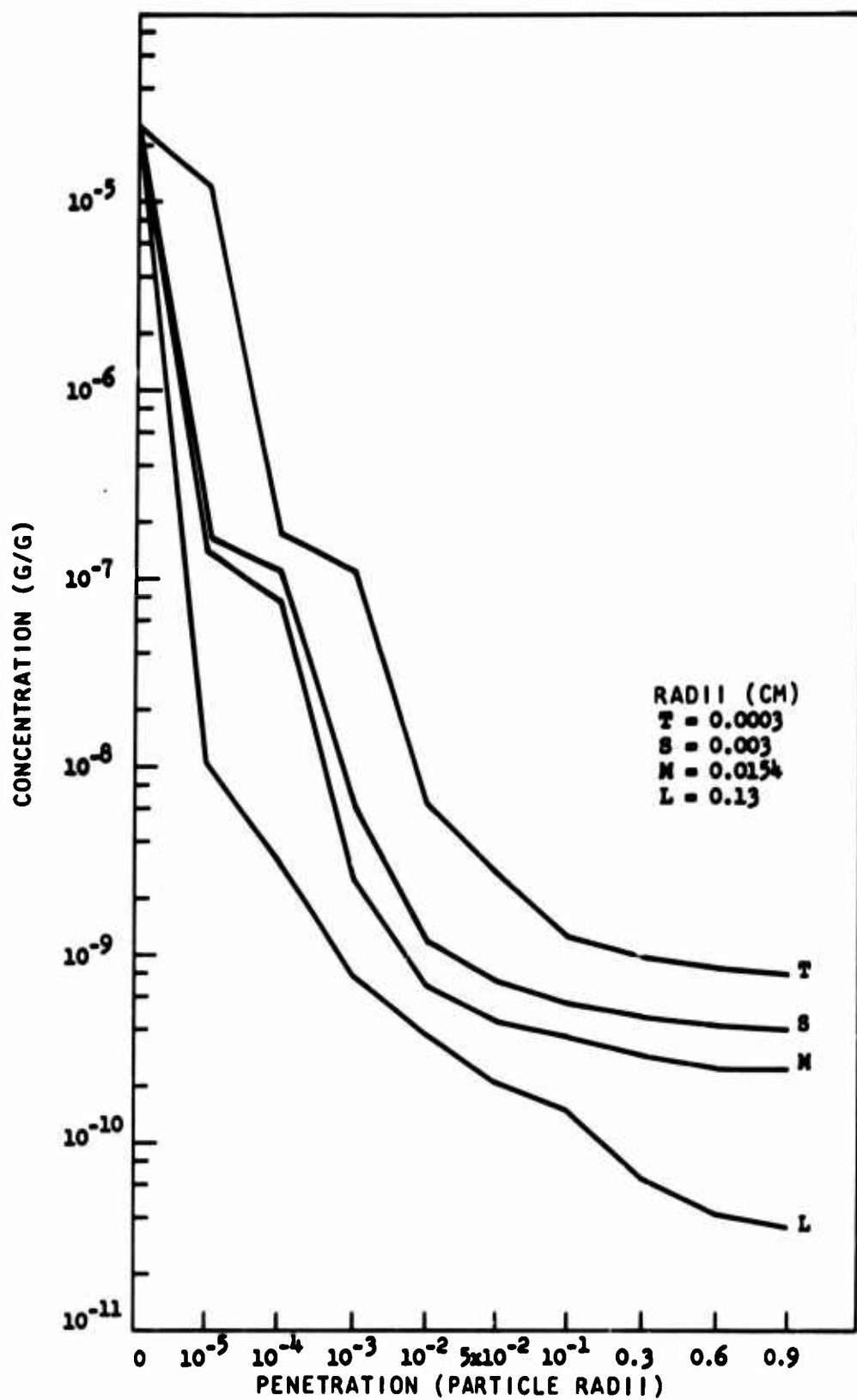


Fig. B.6--Cesium-137 concentration profiles at 900°K for standard particle size and standard detonation

The 900°K profiles for the 95 chain are very simple. They show only small deviations from a flat profile for rubidium in the S, M, and L particles and for the other fission products just in the L particles. The 900°K profiles for the 137 chain are structurally more interesting. The distribution of tellurium within the standard particles at this temperature is shown in Fig. B.4. Calculated tellurium concentrations span eight orders of magnitude in the L particles and five orders of magnitude in the T particles. The concentrations have been drawn as a continuous curve in these diagrams as an aid to the reader and are not to be used in interpolating. The tellurium profiles, then, are characteristic of a moderately volatile fission product (1% condensed at 900°K in this calculation) with a moderately high Henry's law temperature coefficient.

The iodine and xenon profiles (shown in Fig. B. 5) are even more interesting, since they exhibit maxima and minima as a function of radius and particle size. The sharp maxima in the iodine curves can be attributed to absorbed tellurium decay and subsequent diffusion and vaporization of the resulting iodine. The maxima in the xenon curves can be attributed to absorbed iodine decay and diffusion and vaporization of resultant xenon.

The cesium profiles are shown in Fig. B. 6. This set of curves would appear to be exhibiting fine structure that is somewhat dependent on the calculational model. The near-surface behavior of calculated profiles would seem to have an extraneous structure that is a function of the size of the time-temperature steps. The use of shorter time steps should smooth out this profile considerably. However, the general structure of these profiles seems reasonable.

It is interesting to consider the penetration depths used in these mathematical profile calculations. The particle radius $0.0003 \text{ cm} \times 10^{-5}$ fractional penetration gives 0.3 \AA , a value too low on the atomic-size scale to be a credible penetration depth. This can also be said for the 0.0003-cm radius particles at 10^{-4} radius penetration, and the 0.003-cm radius particles at 10^{-5} radius penetration. A value between 15 and 30 \AA , a

borderline penetration, is the next smallest penetration depth plotted. The subsequent minimum value is 130 \AA , a value such that diffusion is reasonable to consider.

A plot of the iodine profiles for the 0.0003-cm radius particles, T , as a function of temperature is shown in Fig. B. 7. These curves demonstrate a general decrease in total iodine loading as the cloud cools. This can be attributed to the expansion of the cloud, high iodine diffusion coefficients, and a low iodine Henry's law temperature coefficient. At the lower temperatures, where iodine is not very mobile, the iodine profile reflects the parent tellurium profile. The difference between the 1100°K and the 900°K profiles is caused by additional tellurium decay to iodine.

This orientation investigation demonstrates the effects of condensed state diffusion in a fallout calculational model embodying this phenomenon. It is interesting to compare this system with the Miller model, where diffusion is deemed infinitely fast above 1673°K and negligibly slow below this temperature. For the case of the highly absorbed nuclide chain, the only noticeable difference is that the calculations for the larger particles in the diffusion-controlled model suggest that equilibrium conditions may not be attained by these particles during fallout formation. Equilibrium conditions are assumed by Miller. In the case of a volatile chain, the diffusion model predicts an absorption behavior which varies with particle size. Miller's model assumes no absorption difference with particle size. In the diffusion model, cooling rate will slightly affect absorption, while in Miller's model it will affect absorption only to the extent that this quantity interacts with fission product decay. Radial concentration gradients are predicted within a fallout particle with the diffusion model, while with Miller's model there are no concentration gradients within a particle, only at the surface of the particle. It seems reasonable to state that the diffusion model provides a more revealing and perhaps a more accurate calculational tool for considering fallout. It is, however, a limited model, and the assumptions underlying the development of the model should not be ignored.

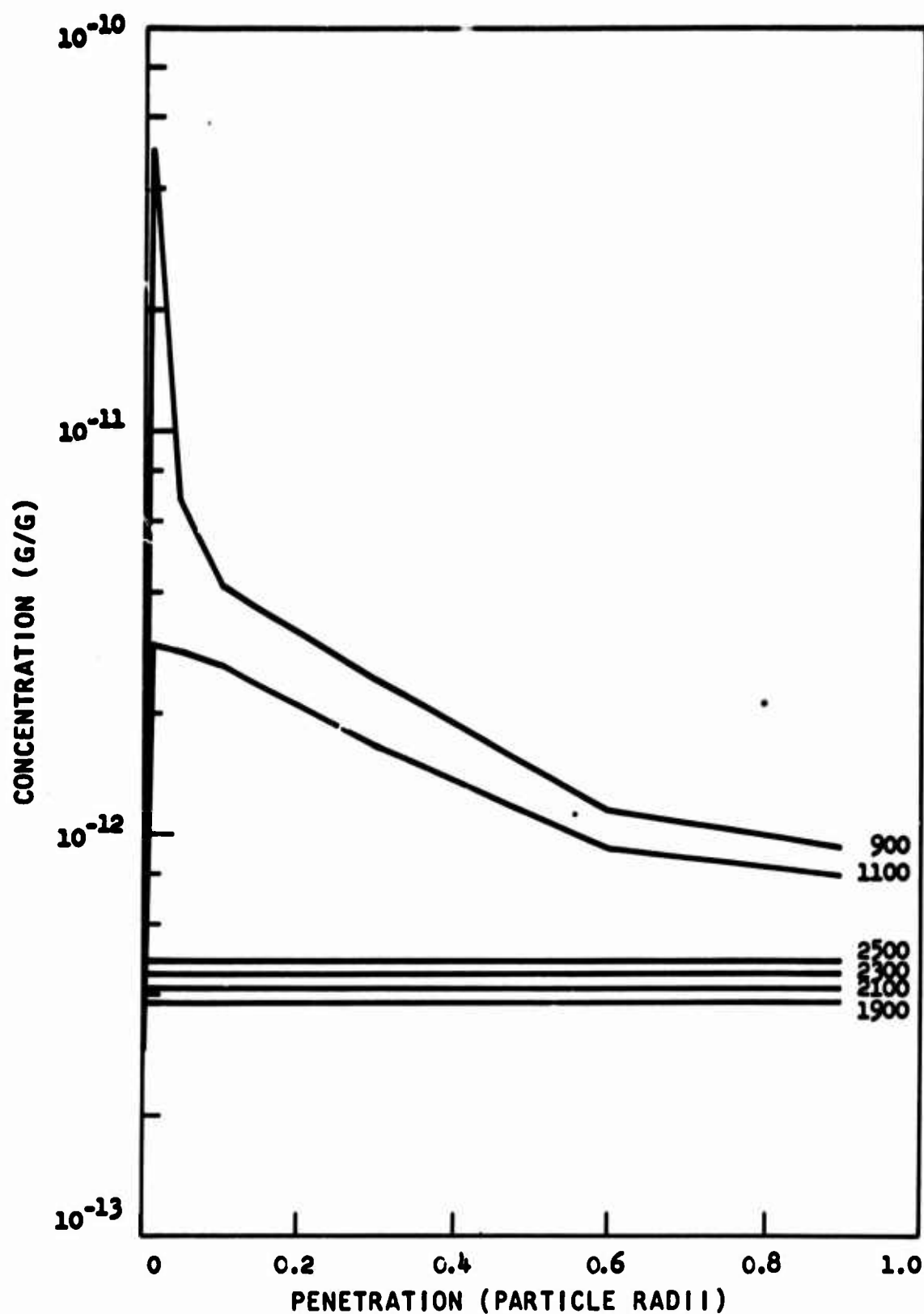


Fig. B. 7--Iodine-137 concentration profiles as a function of final temperature for the 0.0003 cm size particles and the standard detonation

APPENDIX C
CONTROL CARD FORMATS

For identification only

Word	1-12	13	14		
Column	1-22	23-75	77-99		
Format	12A6	13	A4		
Card 1	Case title: may be any set of characters desired	Numerical case designation (564 has been used)	Sub-case designation (for identification)		
Symbol	NTITLE	NCS1	NCS2		

LC ≤ 6
IR ≤ 30
IDPTH ≤ 11

Word	1	2	3	4	5	6
Column	1-5	6-10	11-15	16-20	21-30	31-40
Format	15	15	15	15	F10.0	F10.0
Card 2	Length of chain (number of isotopes)	Number of particle sizes	If equal to 0, do not calculate long term results; if equal to 1, do calculate results	Number of depths to calculate concentrations (for profiles)	Yield of device (in KT) used in calculating time-temperature distribution	Yield of device (in KT) used in calculating time-temperature distribution
Symbol	LC	IR	ILC	IDPTH	YKT	BKT

If IDPTH = 0, this card is not present
 $0 < Q(1) \leq 1.0$

Word	1	2	3		
Column	1-10	11-20	21-30		
Format	F10.0	F10.0	F10.0		
Card 2a	First distance from center (in radius units) for concentration calculation	Second distance	Third distance	Etc.	Note: Q(0) = 1 gives surface, Q(0) = 1/2 gives half way into particle, etc.
Symbol	Q(1)	Q(2)	Q(3)		

Word	1	2	3	4	5	6
Column	1-6	7-16	17-26	27-36	37-46	47-56
Format	A6	F10.0	F10.0	F10.0	F10.0	F10.0
Card	Name of isotope	Molecular weight of isotope (in g/mole)	Initial yield of isotope (in g/10 ⁶ fissions)	Constants used to calculate Henry's law constants for this isotope: $\text{Log } H = \text{HC1} + \text{HC2}/T$	Constant used in diffusion coefficient calculation	
Symbol	NAME(L)	WMOL(L)	YIEL	HC1(L)	HC2(L)	DC(L)

There are LC of card type 3, the last isotopes being first

Word	7	8
Column	57-66	67-76
Format	F10.0	F10.0
Card	Constant used in diffusion coefficient calculation	The half-life of this isotope (in seconds)
Symbol	DC2(L)	HL(L)

Word	1	2	3
Column	1-10	11-20	21-30
Format	F10.0	F10.0	F10.0
Card	The starting (highest) temperature for beginning calculations	The final (lowest) temperature for calculations	The incremental temperature
Symbol	HTMP	ETMP	TEMPV

All temperatures are in °K

Note:

$$\frac{\text{HTMP} - \text{ETMP}}{\text{TEMPV}} \leq 40$$

There are 28 of card
type 5
 $0.0 < PW(K) \leq 1.0$

Word	1	2			
Column	1-10	11-20			
Format	F10.0	F10.0			
Card 5	The radius (in cm) of a particle size	The fraction of soil contained in this particle size			
Symbol:	R(K)	PW(K)			

Word	1				
Column	1-16				
Format	E16.8				
Card 6	Total soil weight contained (in g/Kt)				
Symbol	TWGT				

Word					
Column					
Format					
Card					
Symbol					

APPENDIX D

SAMPLE OUTPUT AND SUBPROGRAM LISTINGS

INPUT DATA

SAMPLE CASE, NORMAN CODE.

LENGTH OF CHAIN = 4
 DEVICE YIELD = .10000000+03 KY
 YIELD = .10000000+03(FOR TIME-TEMP DISTRIBUTION)

ISOTOPE PARAMETERS

NAME	MOLECULAR WEIGHT (G/MOLE)	INITIAL YIELD (ATOMS/10,000 FISSIONS)	MC1	MC2	DC1	DC2	HALF LIFE (SECONDS)
CS	137.	6.0	6.600	17300.0	5.570	20500.0	.40
XE	137.	114.0	4.100	700.0	9.100	20500.0	234.00
I	137.	252.0	3.400	1000.0	7.290	22500.0	24.40
TE	137.	172.4	9.200	11400.0	3.300	15600.0	3.00

STARTING TEMPERATURE = 2900. DEG. KELVIN
 FINAL TEMPERATURE = 900. DEG. KELVIN
 TEMPERATURE INCREMENT = 200. DEG. KELVIN
 TOTAL PARTICLE WEIGHT = 8.50000000+07 G/KY

PARTICLE PARAMETERS & PARTICLE SIZES

RADIUS (CM)	WEIGHT (G)
.000300	3.23000000+07
.003000	2.45819900+09
.015400	5.11599900+09
.130000	8.92500000+03

TIME-TEMPERATURE DISTRIBUTION: 10 STEPS.

TIME INCH	TEMP
5.10650	.75626
5.89304	.81683
6.74542	.88794
7.67571	.97263
8.69962	1.07519
9.83019	1.20136
11.12051	1.36267
12.58839	1.57309
14.30521	1.86057
16.37407	2.27715
	900.0

START TIME FOR CALCULATION OF SURFACE CONCENTRATIONS IS 4.7204 SEC

YIELDS, IN GRAMS, ADJUSTED TO START TIME.

ISOTOPE	YIELD
CS	2.51545820+08
XE	4.69730700+01
I	1.04952669+02
TE	1.65439360+01

DIFFUSION COEFFICIENTS (LINE ONE) AND HEAVY'S LAW CONSTANTS (LINE TWO)

TEMP	CS	XE	I	TE
2700.0	9.49308720-03 1.55809006+00	1.92834660-01 0.93011950+03	9.05037790-02 2.64924034+03	3.32829430-03 6.75506030+04
2500.0	2.34822680-03 4.76630100-01	3.16227760-02 6.60693380+03	1.94938440-02 2.51184630+03	1.14415353-03 3.01995170+04
2300.0	4.53496220-04 1.19745950-01	3.76669890-03 6.24672120+03	3.21655760-03 2.31855480+03	3.29143000-04 1.17372180+04
2100.0	6.42828680-05 2.30093700-02	3.02659150-04 5.84341350+03	3.76456110-04 2.10770350+03	7.43752740-05 3.51024060+03
1900.0	6.03290260-06 3.12618540-03	1.42112250-05 5.38987790+03	2.40475440-05 1.47795070+03	1.22477434-05 9.76353650+02
1700.0	3.24471440-07 2.65173050-04	3.24911180-07 4.87792640+03	1.13424237-06 1.62641340+03	1.32901372-06 1.51477793+02
1500.0	8.00446510-09 1.16591420-05	2.71247340-09 4.29866190+03	1.94908440-06 1.35935630+03	7.94324230-07 2.15443490+01
1300.0	6.32075380-11 1.96023260-07	5.19259860-12 3.64366500+03	9.50006800-11 1.07341880+03	1.94526240-06 1.32762050+00
1100.0	8.58294790-14 7.45980130-10	1.02115328-15 2.90328060+03	6.44624100-14 7.77673650+02	1.31274937-11 2.96930850-02
900.0	6.19753360-18 2.36659030-13	4.52934420-21 2.10001420+03	1.44964470-16 4.65527320+02	9.25113613-15 1.22712520-04

SURFACE CONCENTRATIONS IN G/G

TEMP	TIME	CS	XE	I	TE
2700.0	5.106+00	1.97850050-11	9.27948080-14	5.12442020-13	3.60449230-15
2500.0	5.693+00	5.17861580-11	8.75030070-14	4.76090160-13	5.43337400-15
2300.0	6.745+00	1.33402590-10	4.22951770-14	4.39956150-13	1.65762369-14
2100.0	7.676+00	2.09640170-10	7.72236250-14	4.04667760-13	2.22311140-14
1900.0	8.700+00	4.14980540-10	7.23277880-14	3.71628470-13	5.71540330-14
1700.0	9.833+00	5.75703290-10	6.76943160-14	3.41194250-13	1.93292430-13
1500.0	1.112+01	1.13076421-09	6.34630980-14	3.14446110-13	9.67553720-13
1300.0	1.259+01	7.31660820-09	5.96815490-14	2.94612200-13	0.67935350-12
1100.0	1.431+01	1.93220210-07	5.74340050-14	2.44393330-13	1.94753210-10
900.0	1.637+01	2.49293130-05	5.72266180-14	2.93608840-13	2.05933540-03

AMOUNT OF MATERIAL IN THE GAS PHASE
(IN GRAMS)

ISOTOPE

TEMP	TIME	CS	XE	I	YE
2700.0	5.100+00	2.34744740+00	4.89722820+01	1.44944313+02	1.45+30050+01
2500.0	5.893+00	2.19064010+00	5.10934650+01	1.45890554+02	1.55700241+01
2300.0	6.745+00	1.05912151+00	5.33933620+01	1.05944048+02	1.23924532+01
2100.0	7.676+00	7.88477610+01	5.58932070+01	1.05697472+02	1.05013717+01
1900.0	8.700+00	1.94927950+01	5.86129640+01	1.04930746+02	0.38758710+03
1700.0	9.833+00	2.34709870+02	6.15831460+01	1.03619377+02	0.54203330+03
1500.0	1.112+01	3.15577690+03	6.40426430+01	1.01727363+02	4.95466360+03
1300.0	1.259+01	4.69906200+04	5.84431020+01	9.32629550+01	3.61436760+03
1100.0	1.431+01	6.25290240+05	7.24614900+01	9.54624550+01	2.50307570+03
900.0	1.637+01	3.01224350+06	7.70039060+01	9.19044860+01	1.61952273+03

AVERAGE CONCENTRATIONS PER PARTICLE SIZE
AT FINAL TEMPERATURE 900. DEG CELSIUS

ISOTOPE

PARTICLE RADII
(IN CM)

	CS	XE	I	YE
.00030	3.59673050+09	2.06275100+13	6.70915050+12	4.25040330+11
.00300	8.30925760+10	1.52171700+13	1.20506492+12	4.40337110+12
.01540	4.20978970+10	1.49355310+13	5.17927000+13	6.60214940+13
.13000	1.34016040+10	1.70123950+13	3.62420370+13	1.04160273+13
AVERAGE	5.21472400+10	1.52566390+13	7.24713320+13	1.96332370+12

P P O F I L E P O I N T S

CONCENTRATIONS AT VARIOUS DEPTHS
AT FINAL TEMPERATURE 900. DEG KELVIN

*** CS ISOTOPE ***

PARTICLE RADIUS	.99000	.90000	.80000	.70000	.50000	DEPTH (R/A)
.000300	6.32445-09	1.33118-09	1.05533-09	1.01280-09	9.24212-10	
.003000	1.25965-09	5.73416-10	5.15717-10	4.86937-10	3.44444-10	
.015400	7.21825-10	3.92768-10	3.40076-10	3.04320-10	2.71060-10	
.130000	3.47207-10	1.51910-10	9.32232-11	6.93712-11	4.72192-11	

*** XC ISOTOPE ***

PARTICLE RADIUS	.99000	.90000	.80000	.70000	.50000	DEPTH (R/A)
.000300	2.31018-13	2.34434-13	2.14135-13	1.92633-13	1.65670-13	
.003000	2.28507-13	1.44232-13	1.53962-13	1.41480-13	1.43079-13	
.015400	1.56731-13	1.44820-13	1.46932-13	1.49524-13	1.52106-13	
.130000	1.45673-13	1.44834-13	1.71597-13	1.76356-13	1.80975-13	

*** I ISOTOPE ***

PARTICLE RADIUS	.99000	.90000	.80000	.70000	.50000	DEPTH (R/A)
.000300	4.93079-11	4.19106-12	3.27276-12	2.44562-12	1.34946-12	
.003000	3.67355-12	7.10290-13	5.46660-13	4.54748-13	4.04552-13	
.015400	1.00400-12	3.78573-13	3.49723-13	3.34723-13	3.33912-13	
.130000	3.83461-13	3.35447-13	3.39240-13	3.42618-13	3.46459-13	

*** TE ISOTOPE ***

PARTICLE RADIUS	.99000	.90000	.80000	.70000	.50000	DEPTH (R/A)
.000300	8.66849-11	3.15110-12	2.35084-12	1.64763-12	7.47300-13	
.003000	2.88242-12	2.05907-13	1.14677-13	6.60401-14	4.13749-14	
.015400	4.42426-13	2.71600-14	1.33915-14	8.45334-15	5.83541-15	
.130000	2.93181-14	2.00482-15	9.73195-16	6.54726-16	4.22769-16	

SUMMARY OF RESULTS AT FINAL TEMP 900. DEG KELVIN

ISOTOPE

	CS	XE	I	TE
AMT IN GAS PHASE	3.6122350-06	7.70039060+01	9.19648660+01	1.61962273+00
AMT IN SOLID PHASE	6.43251550+00	1.29651855-03	6.16006330-03	1.67307940-02
TOTAL	6.43251920+00	7.70032020+01	9.19110950+01	1.63635352+03
YIELD AT FINAL TIME	6.43252020+00	7.70052020+01	9.19110950+01	1.63635352+00
DIFFERENCE	-9.53674320-07	0.00000000	-2.66102290-06	-1.39011610-03

LONG-TERM RESULTS FOR CS ISOTOPE

PARTICLE RADIUS (CM)	AVERAGE CONCENTRATION DUE TO SOLID'S DECAY (G/G)	TOTAL AVERAGE CONCENTRATION (INCLUDES GAS PHASE) (G/G)	TOTAL AMOUNT OF CS IN PARTICLE (G)
.00030	5.64615-93-08	.5256560-07	1.66170734+01
.00300	8.36646370-10	6.57289560-09	1.12310917+02
.01540	4.22515473-10	9.16776290-09	4.60116240+01
.13000	1.34633550-10	1.17062609-09	1.04474537+00

01 FOR NORMAN

COMPILATION BY UNIVAC 1103 FORTRAN-IV JATED. 11 NOV 1966 F4008

THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:05:57

MAIN PROGRAM ENTRY POINT 000000

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CODE 002101
0000 *DATA 023461
0002 *BLANK 001676
0003 SING 000023
0004 91 023160
0005 INLOOP 000001

EXTERNAL REFERENCES (BLOCK, NAME)

0006 MARGIN
0007 INITIAL
0010 EXP
0011 DIFFUS
0012 ALO610
0013 BCALC
0014 PROFIL
0015 DELTA
0016 FINAL
0017 DUMP
0020 HEAR25
0021 N0005
0022 N1015
0023 N1025
0024 N5TOP5

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	001161	10L	0001	002020	1000L	0001	002085	1001L	0001	000713	101L	0001	023377	1050E
0000	023067	1075F	0000	023114	1076F	0000	001153	111L	0001	000723	111L	0001	021145	12L
0000	023122	1200F	0000	023152	1201F	0000	023213	1202F	0000	023220	1203F	0000	023245	1215F
0000	023254	1208F	0000	023265	1207F	0000	023273	1208F	0000	023304	1209F	0000	020733	121L
0000	023312	1210F	0000	023320	1211F	0000	023352	1212F	0000	023374	1213F	0000	020013	1244
0001	000021	1276	0001	001137	13L	0001	000743	131L	0001	000335	1325	0001	001131	14L
0001	000051	1416	0001	000130	1556	0001	000141	1606	0001	000154	1653	0001	000157	1753
0001	001076	18L	0001	001107	19L	0001	000213	2026	0001	000300	21L	0001	000231	2115
0001	000245	2146	0001	000056	22L	0001	000266	2216	0001	000333	2363	0001	000155	24L
0001	001700	232L	0001	000401	2543	0001	000424	2606	0001	000457	2703	0001	000395	28L
0001	000535	3046	0001	000555	3116	0001	000634	3266	0001	000700	3345	0001	001324	3716
0001	001044	3766	0001	000753	40L	0001	000310	401L	0001	001254	4100	0001	001304	4553
0001	001332	47L	0001	001175	5L	0001	000362	501L	0001	000365	502L	0001	001322	5035
0001	001234	503L	0001	001237	504L	0001	001431	5106	0001	001441	5163	0001	001361	5275

NORMAN --- MAIN PROGRAM

0001	001470	5346	0001	001472	5376	0001	001514	5476	0001	001535	5615	0001	001545	5655
0001	001553	5736	0001	001550	600L	0001	001507	6016	0001	000020	601L	0001	000007	5612
0001	001206	602L	0001	001572	6056	0001	001615	6176	0001	000043	6335	0001	001652	6475
0001	001660	6455	0001	001666	6526	0001	001725	6656	0001	001734	6745	0001	001745	7425
0001	001756	7106	0001	001770	7166	0001	002001	7245	0001	002266	A	0002	001334	AC
0002	R 000000	ALU610	0002	R 001626	AT4	0000	Q 017036	ADAV	0001	Q 000374	AVCJ4	0001	Q 022763	II
0000	R 023002	BDF	0000	R 023003	QDF1	0000	Q 023004	BDS	0001	Q 022755	JA	0000	R 022763	II
0000	R 017394	COAC	0004	R 003000	OCY	0000	R 000716	DOH	0002	Q 000374	ZFC	0003	Q 017130	NYE
0001	R 000300	UIFFUS	0000	R 022752	DRK	0000	Q 022751	DT	0003	Q 022751	STEL4	0000	Q 022764	3VER41
0000	R 022753	DVD	0010	R 000000	EXP	0000	Q 000660	F4	0000	Q 000366	GLS	0002	Q 000754	HE1
0000	I 000360	I	0003	I 000007	IDPTH	0000	I 022741	IEPR	0003	I 000006	ILS	0003	I 000001	IS
0000	I 022767	ISUB	0000	I 022772	II	0000	I 022744	J	0003	I 022746	K	0003	I 022765	KKA
0000	I 022762	KRIK	0005	I 000000	L	0003	I 000000	LC	0003	I 022750	LCC	0003	I 022743	---
0000	I 022756	KWK	0000	I 022742	II	0002	I 000360	NAE	0003	I 000303	NCST	0003	I 000006	NCST
0000	I 022767	NEL	0000	I 022771	NEP	0000	I 022770	NET	0001	I 022757	IT	0003	I 022754	ITAE
0003	I 000002	NTOT	0000	I 022774	NI2	0000	I 022775	NI22	0003	I 022775	II	0003	I 022776	IN
0000	I 022777	NS	0000	I 023000	OB	0000	Q 023001	PDFLT	0014	R 000000	PROFIL	0003	Q 000010	---
0002	R 001342	R	0000	R 022750	PCST	0000	Q 017014	SOLIJ	0000	Q 022745	SUM	0003	Q 000006	50231
0002	R 001506	I	0002	R 001556	TEMP	0000	Q 017022	TOTAL	0003	Q 00035	TAT	0003	Q 023005	Y1
0000	R 000754	UM	0002	R 001436	VOL	0002	R 000356	WML	0004	Q 023000	W1	0002	R 001400	W1
0002	R 000000	YLD	0000	R 023005	YTY									

*** MAIN PROGRAM FOR NORMAN PROBLEM ***

PROGRAM COMPUTES SURFACE CONCENTRATIONS OF CHAINS OF ISOTOPES.

SUMMARY OF MAJOR VARIABLE NAMES

00100	1.	C	DECAY(I,J,K)	DECAY COEFFICIENT OF ISOTOPE I FROM TIME J TO TIME K.
00100	2.	C	GAST(I)	AMOUNT OF ISOTOPE I IN THE GAS PHASE.
00100	3.	C	AVCON(I,J)	AVERAGE CONCENTRATION OF ISOTOPE I IN PARTICLE SIZE J.
00100	4.	C	PH(I),DOD(I)	DIFFUSION TERMS ASSOCIATED WITH PARTICLE SIZE J.
00100	5.	C	SURCON(I,J)	SURFACE CONCENTRATION OF ISOTOPE I AT TIME J.
00100	6.	C	I(K)	ARRAY OF SUBSCRIPTS DESCRIBING A DECAY PATH.
00100	7.	C	SOLUT(I)	AMOUNT OF ISOTOPE I IN THE SOLID PHASE.
00100	8.	C	CONC(I,J,K)	CONCENTRATION OF ISOTOPE I IN PARTICLE SIZE J AT A RELATIVE RADII (K).
00100	9.	C	Q(K)	ARRAY OF RELATIVE RADII FOR CALCULATING CONC

(SEE SUBROUTINE INITIAL FOR ADDITIONAL VARIABLE DEFINITIONS.)

00101	25.	C	COMMON YLD(6,40),NAE(40),VOL(6),DEC(6,40),HEH(6,40),AK(6),K(30),J
00101	26.	C	/T(30),VOL(40),T(40),TEVP(40),ATM(40)
00103	27.	C	COMMON/SING/LC,IR,NTOT,NCST,NCST,YST,IL6,IDPTH=0
00104	28.	C	COMMON/BI/DCY(6,40,40),BN(6,40)
00105	29.	C	COMMON/TL/DSP7L

NORMAN --- MAIN PROGRAM.

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00106 30. DIMENSION SURCON(6,40),I(6)
00107 31. DIMENSION GAS(6)
00110 32. DIMENSION AVCON(6,30)
00111 33. DIMENSION FNT(30),DOOT(30)
00112 34. DIMENSION UN(6,40,30)
00113 35. DIMENSION SOLID(6),TOTAL(6),DIF(6)
00114 36. DIMENSION AVAV(6)
00115 37. DIMENSION CONC(6,30,11),O(11)
00116 38. DATA KCST/.0820597/
00116 39. C
00116 40. C SUBROUTINE INITIAL READS ALL PARAMETERS FOR THIS CASE
00116 41. C AND PRINTS OUT ALL INPUT.
00116 42. C INITIAL ALSO PREPARES INPUT TO BE COMPATIBLE WITH MAIN PROGRAM
00116 43. C
00120 44. CALL MARGIN(4,62)
00121 45. IERREQ
00122 46. 3 CALL INITIAL
00122 47. C
00122 48. C LOOP 20 FINDS ALL DECAY COEFFICIENTS.
00122 49. C
00123 50. DO 20 NEI,LC
00126 51. DO 20 NEI,NTOT
00131 52. DO 20 J=1,NTOT
00134 53. SUMEQ.
00135 54. IF(J-M)21,22,23
00140 55. 23 DO 24 KEM,J
00143 56. 24 SUMESUM+T(K)
00145 57. 60 TO 21
00146 58. 22 SUMT(J)
00147 59. 21 DCYTH,X,J=EXP(-AR(T)*SUM)
00150 60. 20 CONTINUE
00150 61. C
00150 62. C INITIALIZATION OF PROFILE POINTS AND AVERAGE CONCENTRATIONS.
00150 63. C
00154 64. DO 25 K=1,IR
00157 65. DO 25 L=1,LC
00162 66. IF(IDPTH.EQ.0)50 TO 25
00164 67. DO 26 ISUB=1,ISPTH
00167 68. 26 CONCL,K,ISUB)=0.
00171 69. 25 AVCON(L,K)=0.
00171 70. C
00171 71. C SUBSECTION TO CALCULATE YIELDS FOR ALL TIMES AND ELEMENTS.
00171 72. C YLD(L,J)=YIELD AT TIME J FOR ELEMENT L.
00171 73. C
00174 74. DO 300 J=2,NTOT
00177 75. YLD(L,J)=YLD(L,C,J)=YDCY(LC,CJ=1,J=1)
00200 76. LCC=LC-1.
00201 77. DO 301 L=1,LC
00204 78. 301 YLD(L,J)=YLD(L,J-1)+DCY(L,J-1,J-1)+YLD(L+1,J-1)+(1.-DCY(L+1,J-1,J-1)
00204 79. .17)
00206 80. 300 CONTINUE
00206 81. C
00206 82. C SUBSECTION TO CALCULATE THE MN ARRAY. MN(L,J)=SUM OVER ALL
00206 83. C PARTICLES OF THE HEIGHT OF THE PARTICLES TIMES THE SURFACE

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NORMAN --- MAIN PROGRAM.

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00206 84. C CONCENTRATION RATIO. THE SURFACE CONCENTRATION RATIO IS THE
00206 85. C SOLUTION TO THE DIFFUSION EQUATION, USING AS A DT TERM THE
00206 86. C DIFFUSION COEFFICIENT OF ELEMENT L DURING THE JTH TIME INTERVAL.
00206 87. C
00210 88. DO 400 J=1,NTOT
00213 89. DO 400 L=1,LC
00216 90. DT=DFC(L,J)*DT(J)
00217 91. SUM=0.
00220 92. DO 401 K=1,IR
00223 93. UH(L,J,K)=1.
00224 *DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTegers MAY NOT BE MEANINGFUL.
00224 94. IF(DT*.GE.(1.8*R(K)*.2))GO TO 401
00226 95. UH(L,J,K)=DIFFUS(DT,R(K))
00227 96. 401 SUM=SUM+UH(L,J,K)*DT(K)
00231 97. 400 UH(L,J)=SUM
00231 98. C
00231 99. C SUBSECTION TO CALCULATE THE SURFACE CONCENTRATION (SURCON) FOR
00231 100. C EACH ISOTOPE AT TIME STEP ONE.
00231 101. C
00234 102. DRK=VOL(1)/(RCST*E-P(1))
00235 103. DO 500 L=1,LC
00240 104. IF(ALGLOG(EN(L,1))+ALOG10(DRK).GT.35.) GO TO 501
00242 105. DVO=AMOL(L)*EN(L,1)*DRK*UH(L,1)
00243 106. GO TO 502
00244 107. 501 DVO=1.E37*UH(L,1)
00245 108. 502 CONTINUE
00246 109. IF(DVO)500,1000,500
00251 110. 500 SURCON(L,1)=VLD(L,1)/DVO
00251 111. C
00251 112. C *** MAIN LOOP ***
00251 113. C
00251 114. C CALCULATION OF SURFACE CONCENTRATIONS FOR EACH ISOTOPE AT FACT
00251 115. C TIME.
00251 116. C
00253 117. DO 600 NTIME=2,NTOT
00256 118. DRK=VGLNTIME/(RCST*TEMP(NTIME))
00257 119. DO 600 L=1,LC
00262 120. KRA=LC-[L]
00262 121. C
00262 122. C KRA-1 IS THE NUMBER OF PREDECESSORS CONTRIBUTING TO ISOTOPE L AT
00262 123. C TIME NTIME.
00262 124. C
00263 125. MAK=MINO(KRA,NTIME)
00264 126. NTE=NTIME-1
00265 127. SUM=0.
00266 128. 111750
00266 129. C
00266 130. C LOOP 601 FINDS CONTRIBUTIONS TO ISOTOPE L FROM L AT PRECEDING
00266 131. C TIME STEPS.
00266 132. C
00267 133. DO 601 K=1,NT
00272 134. 112750-K
00272 135. C
00272 136. C SCALE FINDS A DIFFUSION TERM.

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NORMAN --- MAIN PROGRAM.

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00272 137. C
00273 138. CALL BCALC(L,K,I,1,0,000,DIER4)
00274 139. KRIK=K+1
00275 140. I(2)=I(2)-1
00276 141. CALL BCALC(L,KRIK,I,1,41,FI,DIER41)
00277 142. BRES=BI
00300 143. SUM=SUM+ BR+SURCON(L,K)+DCY(L,K,IT)
00301 144. IF(NTIME,NE,NTOT)GO TO 601
00301 145. C
00301 146. C IF FINAL TIME, FIND CONTRIBUTIONS TO AVERAGE CONCENTRATIONS
00301 147. C AND PROFILE POINTS.
00301 148. C
00303 149. C
00306 150. DO 6012 M=1,IR
00310 151. IF(DPTH,EG,DI30 TO 6012
00313 152. DO 6013 ISU3=1,12PTH
00314 153. CONCL=4*(ISU3)*C34C(L,4,ISU3)+DCY(L,K,IT)+SURCON(L,K)+(PROFIL(DIER4
00316 154. *N,NTIME),9(1506))-PROFIL(DIER41,R(V),O(1506)))
00320 155. 6013 CONTINUE
00322 156. 6012 AVCON(L,M)=AVCON(L,M)+DCY(L,K,IT)+SURCON(L,K)+(DJS(41)-FM(41))
00323 157. 601 CONTINUE
00323 158. A=SUM
00323 159. IF(WK,EG,1160 TO 602
00323 160. C
00323 161. C LOOP 603 FINDS CONTRIBUTIONS TO ISOTOPE L FROM ITS PREDECESSORS.
00325 162. C DO 603 N=1,2,N*IK
00325 163. C
00325 164. C VALUE OF NEL IS THE SUBSCRIPT OF A PREDECESSOR OF ISOTOPE L.
00325 165. C
00330 166. SUM=0.
00331 167. NET=NEL-1
00332 168. N2=NEL-L-1
00332 169. C
00332 170. C LOOP 5 FINDS CONTRIBUTIONS FROM ISOTOPE NED AT TIME 122.
00332 171. C DO 5 I1=NET,1
00333 172. C
00336 173. N2=NTIME-I1
00337 174. I(1)=I1
00340 175. B=0.
00340 176. C
00340 177. C THE I ARRAY SPECIFICS THE DECAY PATH FROM IEP AT 122
00340 178. C TO L AT NTIME.
00340 179. C
00341 180. N2=I1-NEL
00342 181. I(2)=1
00343 182. 101 IF(NEL,EG,2160 TO 40
00345 183. N3=N2-I(2)-1
00346 184. I(3)=1
00347 185. 111 IF(NEL,EG,3160 TO 40
00351 186. N4=N3-I(3)-1
00352 187. I(4)=1
00353 188. 121 IF(NEL,EG,4160 TO 40
00355 189. N5=N4-I(4)-1
00356 190. I(5)=1

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NORMAN --- MAIN PROGRAM.
00357 191. 131 IF (NEL.EQ.5) GO TO 40
00361 192. N5=N5-I(5)-1
00362 193. I(6)=1
00363 194. C
00362 195. C DELTA FINDS THE DECAY TERM ASSOCIATED WITH THIS PATH.
00362 196. C
00363 197. C 40 CALL DELTA(NEL,NTIME,I,PDDEL)
00363 198. C
00363 199. C BCALC FINDS THE DIFFUSION TERMS ASSOCIATED WITH THIS PATH.
00363 200. C
00364 201. CALL BCALC(NEL,NTIME,I,1,BDF,DOO,DTER4)
00365 202. CALL BCALC(NEL,NTIME,I,0,BDF,1,FN,DTER4)
00366 203. IF (NTIME.NE.NTOT) GO TO 19
00366 204. C
00366 205. C AT THE FINAL TIME, FIND AVERAGE CONCENTRATION AND PROFILE POINT
00366 206. C CONTRIBUTIONS.
00366 207. C
00370 208. DO 18 N21,NR
00373 209. IF (IDPTH.EQ.0) GO TO 18
00375 210. DO 18O ISUB=1,1DPTH
00400 211. CUNC(L,N,ISUB)=CUNC(L,N,ISUB)+PDDEL*SURCON(NEP,N2P)*(PI*PI*INTER4
00400 212. *R(N)*G1SUB)-PROFIL(DYER4,R(N)*G1SUB))
00401 213. 18O CONTINUE
00403 214. 18 AVCON(L,N)=AVCON(L,N)+PDDEL*SURCON(NEP,N2P)*(DOO(DJ)+I(N))
00405 215. 19 B36=B36+3DF1
00405 216. C
00405 217. C B IS THE SUM OF ALL CONTRIBUTIONS FOR THESE STATES.
00405 218. C
00406 219. C
00407 220. B=B+806*PDDEL
00410 221. GO TO (5,10,11,12,13,18),NEL
00411 222. 14 * (6)=1(6)+1
00414 223. IF (I(6)=46) 40,40,13
00415 224. 13 I(5)=1(5)+1
00420 225. IF (I(5)=45) 13,13,12
00421 226. 12 I(4)=1(4)+1
00424 227. IF (I(4)=44) 12,12,11
00425 228. 11 I(3)=1(3)+1
00430 229. IF (I(3)=43) 11,11,10
00431 230. 10 I(2)=1(2)+1
00434 231. IF (I(2)=42) 10,10,16
00435 232. 16 B=B+SURCON
00437 233. 5 SURCON=3
00441 234. 603 A=A+SUM
00443 235. 602 IF (ALOG10(NTIME/NTOT)+ALOG10(DO0)*G1,N5,1) GO TO 503
00444 236. DVO=DNK+XOL(L)*HEN(L,NTIME)+XN(L,NTIME)
00445 237. GO TO 504
00446 238. 503 DVO=1.E37*XN(L,NTIME)
00447 239. 504 CONTINUE
00452 240. IF (DVO) 666,1001,666
00453 241. T1=DVO-XN(L,NTIME)
00454 242. SURCON(L,NTIME)=T1/Y7DVO
00455 243. IF (NTIME.NE.NTOT) GO TO 600
00457 244. DO 47 N21,NR

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NORMAN --- MAIN PROGRAM.	
00462 245.	IF (IDPTH.EQ.0) GO TO 47
00464 246.	DO 470 ISUB=1, IDPTH
00467 247.	CONC(L,M,ISUB)=CONC(L,M,ISUB)+SURCON(L,NTOT)*PROFIL(DFC(L,NTOT))*T(
00467 248.	NTOT)*R(M)/3(ISUB)
00470 249.	470 CONTINUE
00472 250.	47 AVCON(L,M)=AVCON(L,M)+SURCON(L,NTOT)*DPI(L,NTOT,M)
00474 251.	600 CONTINUE
00474 252.	C
00474 253.	C
00474 254.	C
00474 255.	C
00474 256.	C
00474 257.	C
00477 258.	WRITE(6,1075) MCS1,MCS2,NAME(L),L=1,LC
00507 259.	DO 1090 J=1,NTOT
00512 260.	1090 WRITE(6,1076) TEMP(J),ATM(J),SURCON(L,J),L=1,LC
00512 261.	C
00512 262.	C
00512 263.	C
00523 264.	WRITE(6,1200) MCS1,MCS2,NAME(L),L=1,LC
00533 265.	DO 80 J=1,NTOT
00536 266.	DO 81 L=1,LC
00541 267.	81 GAS(L)=SURCON(L,J)*HE(L,J)*VOL(J)*MOL(L)/(MCS1*TEMP(J))
00543 268.	80 WRITE(6,1076) TEMP(J),ATM(J),GAS(L),L=1,LC
00543 269.	C
00543 270.	C
00543 271.	C
00554 272.	WRITE(6,1201) MCS1,MCS2,TEMP(NTOT),NAME(L),L=1,LC
00565 273.	DO 43 J=1,IR
00570 274.	43 WRITE(6,1202) R(J),AVCON(L,J),L=1,LC
00570 275.	C
00570 276.	C
00570 277.	C
00600 278.	LOOP 88 FINDS SUMMARY RESULTS.
00603 279.	DO 88 L=1,LC
00604 280.	SOLID(L)=0.
00607 281.	DO 89 K=1,IR
00611 282.	89 SOLID(L)=SOLID(L)+AVCON(L,K)*WT(K)
00612 283.	AVAV(L)=SOLID(L)/IR
00613 284.	TOTAL(L)=SOLID(L)+GAS(L)
00615 285.	88 DIF(L)=(TOTAL(L)-VOL(L,NTOT))
00623 286.	WRITE(6,1210) (AVAV(L),L=1,LC)
00625 287.	IF (IDPTH.EQ.0) GO TO 252
00625 288.	WRITE(6,1211) MCS1,MCS2,TEMP(NTOT)
00625 289.	C
00625 290.	C
00632 291.	C
00635 292.	DO 250 L=1,LC
00644 293.	WRITE(6,1212) NAME(L),TOTAL(K)=1, IDPTH
00647 294.	DO 251 K=1,IR
00657 295.	251 WRITE(6,1213) R(K),CONC(L,K),L=1, IDPTH
00657 296.	250 CONTINUE
00657 297.	C
00657 298.	C
00657 299.	C
00657 300.	PRINT SUMMARY RESULTS.

NORMAN --- MAIN PROGRAM

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00661 299. 252 WRITE(6,1204)TEMP(NTOT),NCS1,NCS2,(NAME(L),L=1,LC)
00672 300. WRITE(6,1205)(GAS(L),L=1,LC)
00700 301. WRITE(6,1206)(SOLID(L),L=1,LC)
00706 302. WRITE(6,1207)(TOTAL(L),L=1,LC)
00714 303. WRITE(6,1208)(VLD(L),L=1,LC)
00722 304. WRITE(6,1209)(DIF(L),L=1,LC)
00730 305. IF(ILE.EQ.0)GO TO 3
00732 306. CALL FINAL(AVCON,GAS,R,NT,NAME(1))
00733 307. GO TO 3
00733 308. C
00733 309. C
00733 310. C
00734 311. 1000 WRITE(6,1050)NAME(L),NMOL(L),HEM(L,1),NM(L,1),T(1),TEMP(1),VOL(1)
00745 312. CALL DUMP
00746 313. 1001 WRITE(6,1050)NAME(L),NMOL(L),HEM(L,NTIME),NM(L,NTIME),T(NTIME),TE4
00746 314. XP(NTIME),VOL(NTIME)
00757 315. CALL DUMP
00757 316. C
00757 317. C
00757 318. C
00760 319. 1050 FORMAT(1H0,5X,35H*** ERROR: PROGRAM CANNOT CONTINUE./10X,20HTHE SUR
00760 320. FACE CONCENTRATION OF GAS,1X,12HIS INFINITE./15X,19HMOLECULAR WEI
00760 321. GHT = ,E16.8/15X,23HWEIGHTS LAW CONSTANT = ,E16.8/15X,54HIN = ,E10.
00760 322. X8/15X,17HINFINITE INCRE ENT = ,E16.8/15X,14HTEMPERATURE = ,F9.1/15X,15
00760 323. XH VOLUME OF CLOUD = ,E16.8)
00761 324. 1075 FORMAT(1H0,50X,31H SURFACE CONCENTRATIONS IN U/G ,15X,9H CASE NO. ,
00761 325. /13,1H,,A9/28X,7HISOTOPE//13X,4HTEMP,6X,4HTIME,6X,46,5(13X,46))
00762 326. 1076 FORMAT(1X,7,1,2X,1P8,3,6(13X,1P16,8))
00763 327. 1200 FORMAT(1H1,48X,35H OUTPUT OF MATERIAL IN THE GAS PHASE,61X,10HIN G
00763 328. ,RANST30X,9H CASE NO. ,13,1H,,A9/28X,7HISOTOPE//13X,4HTEMP,6X,4HTIME
00763 329. , ,9X,46,5(13X,46))
00764 330. 1201 FORMAT(1H1,62X,40H AVERAGE CONCENTRATIONS PER PARTICLE SIZE,14X,9H C
00764 331. ASE NO. ,13,1H,,A9/49X,21HAT FINAL TEMPERATURE ,F5.0/11H DEG KELVI
00764 332. ,N7/28X,7HISOTOPE//2X,15H PARTICLE RADIUS,7H(1X C9)13X,46,5(13X,
00764 333. ,46))
00765 334. 1202 FORMAT(1H1,41X,33H SUMMARY OF RESULTS AT FINAL TEMP ,F5.0/11H DEG K
00766 335. 1204 FORMAT(1H1,41X,33H SUMMARY OF RESULTS AT FINAL TEMP ,F5.0/11H DEG K
00766 336. ,ELVT,10X,9H CASE NO. ,13,1H,,A9/28X,7HISOTOPE//26X,46,5(13X,46))
00767 337. 1205 FORMAT(1H0,17H AVERAGE IN GAS PHASE,6(13X,1P16,8))
00770 338. 1206 FORMAT(1H0,17H AVERAGE IN SOLID PHASE,1X,1P16,8,5(13X,1P16,8))
00771 339. 1207 FORMAT(1H0,54H TOTAL,12X,6(13X,1P16,8))
00772 340. 1208 FORMAT(1H0,54H YIELD AT FINAL TIME,1X,1P16,8,5(13X,1P16,8))
00773 341. 1209 FORMAT(1H0,10H DIFFERENCE,7X,6(13X,1P16,8))
00774 342. 1210 FORMAT(1H0,5X,7H AVERAGE,5X,6(13X,1P16,8))
00775 343. 1211 FORMAT(1H1,52X,26H R O F I L E P O I N T 5,21X,9H CASE NO. ,13,1H
00775 344. , ,A9/28X,7HISOTOPE//2X,15H PARTICLE RADIUS,7H(1X C9)13X,46,5(13X,
00775 345. ,ERATURE ,F5.0/11H DEG KELVIN)
00776 346. 1212 FORMAT(1H0,5X,7H AVERAGE,5X,6(13X,1P16,8))
00776 347. , ,A9/28X,7HISOTOPE//2X,15H PARTICLE RADIUS,7H(1X C9)13X,46,5(13X,
00777 348. 1213 FORMAT(1H1,52X,26H R O F I L E P O I N T 5,21X,9H CASE NO. ,13,1H
00777 349. , ,A9/28X,7HISOTOPE//2X,15H PARTICLE RADIUS,7H(1X C9)13X,46,5(13X,

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END OF LISTING. 1 *DIAGNOSTIC* MESSAGE(S).

SUBROUTINE INITIAL

01 FOR INITIAL

COMPILATION BY UNIVAC 1106 FORTRAN-IV DATED 11 NOV 1966 F4000
THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:06:04

SUBROUTINE INITIAL ENTRY POINT 001103

STORAGE USED (BLOCK, NAME, LENGTH)

0001	SCODE	001114
0000	DATA	000626
0002	BLANK	001676
0003	SING	000023

EXTERNAL REFERENCES (BLOCK, NAME)

0004	ALOG
0005	DIFFUS
0006	EXP
0007	NRJUS
0010	NIC15
0011	NIC25
0012	NRJUS
0013	NEAP65

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000054	10L	0000	000164	100F	0000	000275	101F	0000	000310	102F	0000	000337	102F
0000	000360	104F	0000	000402	105F	0000	000406	106F	0000	000436	107F	0000	000457	107F
0000	000464	109F	0000	000502	110F	0000	000506	111F	0000	000534	112F	0000	000541	112F
0000	000545	114F	0000	000563	115F	0001	000605	116G	0001	000703	12L	0001	000567	16L
0001	000050	1406	0001	000067	1466	0001	000625	16L	0001	000107	16H9	0001	000565	16L
0001	000606	19L	0000	000162	200UF	0000	000271	2001F	0000	000306	2002F	0000	000343	2003F
0000	000345	2004F	0001	000304	21L	0001	000177	216G	0001	000223	22L	0001	000204	228G
0001	000334	2606	0001	000350	2706	0001	000471	327G	0001	000507	337G	0001	000532	353G
0001	000554	3676	0001	000612	404G	0001	000635	416G	0001	000716	438G	0001	000727	443G
0001	000743	4536	0001	000745	4566	0001	001004	476G	0001	001014	476G	0001	001022	482G
0001	001032	5106	0001	001036	5206	0001	000451	61L	0001	000440	63L	0001	000403	66L
0001	000453	65L	0001	000541	77L	0001	000542	78L	0002	001334	AA	0004	000009	1336
0002	001626	ATM	0000	000131	9RT	0000	000160	CG1	0000	000161	CG1	0000	000124	CI
0000	000150	C2	0003	000192	C3	0000	000125	C4	0000	000322	DC1	0000	000359	DC2
0000	000102	DDP	0002	000374	DPC	0002	000000	DIFFUS	0000	000335	ET07	0005	000000	F47
0000	000006	HC1	0000	000014	MC2	0002	000754	HE1	0000	000336	HL	0000	000154	IL1
0000	000134	HTMP	0000	000132	I	0003	000007	TDPTH	0003	000306	TL5	0003	000001	79
0000	000127	J	0000	000137	K	0000	000156	KK12	0000	000135	L	0003	000000	LC
0000	000157	LCC	0002	000360	NAME	0003	000003	NCS1	0003	000304	NCS2	0000	000110	RTITLE
0003	000002	MTOT	0000	000126	PI	0000	000004	PM	0003	000010	J	0002	000342	7
0002	0001506	I	0002	000156	TEMP	0000	000152	TEMP	0000	000335	TEMP7	0000	000151	TEMP
0000	000141	TIIV	0000	000155	TI	0000	000153	TIEMP	0000	000149	TI61	0003	000005	TYT
0002	0001436	VOL	0002	000356	WVOL	0002	0001400	W1	0000	000000	Y1	0000	000139	YRT

SUBROUTINE INITIAL

0002 R 000000 YLD 0000 R 00015 ZDC 0000 R 000140 ZDT 0000 R 000147 ZSHI 0000 R 000143 ZTI

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00101 1. SUBROUTINE INITIAL
00102 2. COMMON YLD(6,40),HAE(6),FVOL(6),DFC(6,40),HEN(6,40),AK(6),H(30),A
00103 3. /T(30),VOL(40),T(40),TEMP(40),ATM(40)
00104 4. COMMON/SING/LC,IR,NTOT,NC51,NC52,TY,ILG,IDPH,MO
00105 5. DIMENSION YI(6),HC1(6),HC2(6),DC1(6),DC2(6),HL(6),PU(30),DDP(6)
00106 6. DIMENSION Q(11)
00107 7. DIMENSION NTITLE(12)
00108 8. DATA '174.66E37,C4/2.381G26IE-5/,PI/3.14159265/
00109 9. SUBROUTINE READS ALL DATA AND CALCULATES INITIAL INPUTS NEEDED.
00110 10. C
00111 11. C VARIABLE DEFINITIONS
00112 12. C
00113 13. C LC LENGTH OF CHAIN.
00114 14. C YAT YIELD OF DEVICE USED IN CALCULATING YIELDS (IN KT)
00115 15. C BAT YIELD USED FOR CALCULATING VOLUME, WEIGHT, TEMPERATURES,
00116 16. C AND TIME INCRS. (IN KT)
00117 17. C IR NUMBER OF PARTICLES
00118 18. C NAME ARRAY CONTAINING NAMES OF ISOTOPIES.
00119 19. C FVOL ARRAY CONTAINING MOLECULAR WEIGHTS OF ISOTOPIES (IN GRAMS)
00120 20. C VI ARRAY CONTAINING INITIAL YIELDS AT YEO. (IN ATOMS
00121 21. C PER 10,000 FISSIONS)
00122 22. C DFC ARRAY OF DIFFUSION COEFFICIENTS.
00123 23. C HEN ARRAY OF HENRY'S LAW CONSTANTS.
00124 24. C AK ARRAY OF K, WHERE
00125 25. C -LOG(1/2)K*(HALF LIFE)
00126 26. C R ARRAY OF PARTICLE RADII (IN CM)
00127 27. C AT ARRAY OF PARTICLE WEIGHTS (IN GRAMS)
00128 28. C VOL ARRAY OF CLOUD VOLUMES (IN LITERS)
00129 29. C T ARRAY OF TIME INCREMENTS. (IN SEC)
00130 30. C TEMP ARRAY OF TEMPERATURES. (IN DEG KELVIN)
00131 31. C HL ARRAY OF HALF-LIVES. (IN SECONDS)
00132 32. C P2 ARRAY OF PERCENT OF TOTAL WEIGHT PER PARTICLE SIZE.
00133 33. C NTOT TOTAL NUMBER OF TIME TEMPERATURE STEPS.
00134 34. C HTEMP THE STARTING (HIGHEST) TEMPERATURE.
00135 35. C LTEMP THE FINAL (LOWEST) TEMPERATURE.
00136 36. C TCRPV THE INCREMENTAL TEMPERATURE.
00137 37. C Y6GT TOTAL HEIGHT OF PARTICLES.
00138 38. C YIV TOTAL INITIAL VOLUME OF CLOUD.
00139 39. C HC1,HC2 ARRAYS OF CONSTANTS USED IN CALCULATING HENRY'S LAW
00140 40. C CONSTANTS. LOG(HENRY'S LAW) = HC2/TEMP.
00141 41. C DC1,DC2 ARRAYS OF CONSTANTS USED IN CALCULATING DIFFUSION
00142 42. C COEFFICIENTS. LOG(DIFFUSION) = DC2/TEMP.
00143 43. C
00144 44. C READ INPUT DATA AND PRINT ISOTOPE PARAMETERS.
00145 45. C
00146 46. C READ(5,115) (NTITLE(1),J=1,12),NC51,NC52
00147 47. C READ(5,200) LC,IR,ILG,IDPTH,YAT,BAT
00148 48. C IF (IDPTH.EQ.0) GO TO 10

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SUBROUTINE INITIAL
      49.  READ(5,2002) (I(I), I=1, IOPM)
      50.  10 WRITE(6,100) (N(I), I=1, IOPM)
      51.  DO 90 L=1, LC
      52.  READ(5,2001) NAME(L), ZMOL(L), YI(L), HCI(L), HC2(L), DC1(L), DC2(L), HL(L)
      53.  /)
      54.  90 WRITE(6,101) NAME(L), ZMOL(L), YI(L), HCI(L), HC2(L), DC1(L), DC2(L), HL(L)
      55.  /)
      56.  READ(5,2002) HTEMP, ETMP, TEMPV
      57.  READ(5,2003) (R(K), K=1, IR)
      58.  READ(5,2004) TWGT, TIV
      59.  C3=-.546*(IR**(-.373))
      60.  C
      61.  C TEST STARTING TEMPERATURE--- IF SPECIFIED TEMPERATURE IS SUCH
      62.  C THAT ALL F VALUES ARE UNITY, REDUCE STARTING TEMP. BY ONE
      63.  C INCREMENT.
      64.  C
      65.  C 22 ZTEMP=HTEMP-TEMPV/2.
      66.  ZTEMP=HTEMP-TEMPV/2.
      67.  DO 20 L=1, LC
      68.  ZDC=10.*ZMOL(L)-DC2(L)/ZTEMP
      69.  ZDT=ZDC*ZTM
      70.  ZSUX=0.
      71.  20 ZSUM=ZSUM+DIFFUS(ZDT,R(I))
      72.  IF (ZSUM-1.0) 73, 74, 75
      73.  HTEMP=HTEMP-TEMPV
      74.  GO TO 22
      75.  C
      76.  C PRINT WEIGHT, TEMPERATURE AND VOLUME PARAMETERS.
      77.  C
      78.  21 WRITE(6,102) HTEMP, ETMP, TEMPV
      79.  WRITE(6,103) T*ST
      80.  C
      81.  C CALCULATE WEIGHTS PER PARTICLE SIZE AND PRINT.
      82.  C
      83.  T*ST=T*ST*ST
      84.  DO 91 K=1, IR
      85.  91 W(K)=TWGT*PR(K)
      86.  WRITE(6,104) K
      87.  DO 92 K=1, IR
      88.  92 WRITE(6,105) (K, T*ST(K))
      89.  C2=(C*ST)**(-.01)
      90.  C
      91.  C COMPUTE INITIAL TIME (TINT), INCREMENTAL TIMES (T(I)), AND
      92.  C TOTAL TIMES ATN(I).
      93.  C
      94.  TINT=TALOG(HTEMP/(C1*ZTEMP**2))/C3
      95.  J=1
      96.  TEMPL=HTEMP
      97.  64 TTEMP=TEMPL-TEMPV
      98.  TEMP(I)=TEMPL-TEMPV/2.
      99.  T(J)=TALOG(TEMP/TEMPL)/C3
      100.  IF (TTEMP-TEMPV) 101, 102
      101.  60 J=J+1
      102.  IF (J-40) 102, 102, 53

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SUBROUTINE INITIAL

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00315 103.      62 TEXPL=TIMEP
00316 104.      60 TO 64
00317 105.      63 WRITE(6,106)TEMP(40)
00322 106.      NTOT=40
00323 107.      60 TO 65
00324 108.      61 NTOT=J
00325 109.      65 ATN(1)=TINT+T(1)/2.
00326 110.      DO 66 J=2,NTOT
00331 111.      66 ATN(J)=ATA(J-1)+T(J)+T(J-1))/2.
00331 112.      C
00331 113.      C PRINT TIME-TEMPERATURE DISTRIBUTION.
00331 114.      C
00333 115.      WRITE(6,107)NTOT
00336 116.      DO 70 J=1,NTOT
00341 117.      70 WRITE(6,108)ATN(J),T(J),TEMP(J)
00347 118.      WRITE(6,114)TINT
00347 119.      C
00347 120.      C COMPUTE INITIAL YIELDS IN GRAMS.
00347 121.      C
00352 122.      DO 71 L=1,LC
00355 123.      *DIAGNOSTIC* THE LIST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
00355 123.      IF(ML(L).EQ.0.) GO TO 77
00357 124.      AK(L)=-69315/ML(L)
00360 125.      60 TO 78
00361 126.      77 AK(L)=0.
00362 127.      76 YI(L)=C5*WOL(L)*YKT*YI(L)
00363 128.      71 CONTINUE
00363 129.      C
00363 130.      C CALCULATE YIELDS AT START TIME.
00363 131.      C
00365 132.      HLM=1.E38
00366 133.      DO 14 L=1,LC
00371 134.      IF(ML(L).LT.1.E-5) GO TO 14
00373 135.      HLM=AMIN(HLM,ML(L))
00374 136.      14 CONTINUE
00376 137.      HLM=ML/10.
00377 138.      IF(HLM.GT.TINT) HLM=TINT
00401 139.      TTE=HLM
00402 140.      KNUZ=0
00403 141.      19 DO 15 L=1,LC
00406 142.      15 DDP(L)=EXP(-AK(L)*HLM)
00410 143.      LCC=LC-1
00411 144.      16 IF(LC.EQ.1) GO TO 16
00413 145.      DO 73 L=1,LCC
00416 146.      73 YI(L) =YI(L)*DDP(L)+YI(L+1)*(1.-DDP(L+1))
00420 147.      18 YI(LC)=YI(LC)*DDP(LC)
00421 148.      TTE=HLM
00422 149.      IF(TTE.LT.TINT) GO TO 16
00424 150.      IF(KNUZ.EQ.1) GO TO 13
00426 151.      IF(ABS(TTE-TINT).LT.1.E-5) GO TO 13
00430 152.      KNUZ=1
00431 153.      HLM=TINT-TTE+HLM
00432 154.      60 TO 19
00433 155.      13 DO 17 L=1,LC

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SUBROUTINE INITIAL

[illegible]

SUBROUTINE INITIAL

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00541 210. 108 FORMAT(1H,9X,F8.5,6X,F8.5,10X,F7.1)
00542 211. 109 FORMAT(1H,20X,41H,YIELDS, IN GRAMS, ADJUSTED TO START TIME./10X,7H
00543 212. /ISO TOPE,10X,5HYIELD)
00543 213. 110 FORMAT(1H,9X,A6,6X,1PE16.8)
00544 214. 111 FORMAT(1H1,24X,70H,DIFFUSION COEFFICIENTS (LINE ONE) AND HENRY'S LAW
00544 215. /CONSTANTS (LINE TWO),3X,9MCASE NO. ,13,1H,,A2//4X,4HTEMP,2A,6(13X
00544 216. /,A6)/)
00545 217. 112 FORMAT(1H,1X,1X,F9.1,7X,6(3X,1PE16.8))
00546 218. 113 FORMAT(17X,6(13X,1PE16.8))
00547 219. 114 FORMAT(1H,0,9X,56H,START TIME FOR CALCULATION OF SURFACE CONCENTRATI
00547 220. /0.5 IS ,F9.5,4H SEC)
00550 221. 115 FORMAT(12A6,13,1X,A6)
00551 222. RETURN
00552 223. END

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END OF LISTING. 1 *DIAGNOSTIC* MESSAGE(S).

SUBROUTINE FINAL

01 FOR FINAL
 COMPILE BY UHVAC 1108 FORTRAN-IV DATED 11 NOV 1966 F4008
 THIS COMPILE WAS DONE ON 19 DEC 66 AT 21:06:09

SUBROUTINE FINAL ENTRY POINT 000123

STORAGE USED (BLOCK, NAME, LENGTH)

0001	*CODE	000152
0000	*DATA	000345
0002	*BLANK	000000
0003	SING	000006

EXTERNAL REFERENCES (BLOCK, NAME)

0004	NAME
0005	NAME
0006	NAME

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000	000234	100F	0000	000320	101F	0001	000014	107G	0001	000015	113J	0001	000016	118G		
0001	000037	131G	0001	000052	180G	0001	000100	158G	0001	000000	FC	0001	000000	FC		
0000	R	000074	FW	0000	R	000250	GT	0000	I	000233	I	0003	I	000226		
0000	I	000227	K	0000	I	000251	L	0003	I	000300	LC	0003	I	000226		
0003	000002	MTOT	0003	000015	TWT	0000	R	000170	V	0003	I	000232	AV	0003	I	000132

00101	1.	SUBROUTINE FINAL	AVCON(6,30),GAS(6),Z(30),Z(30)	FI 1A0010
00103	2.	DIMENSION	AVCON(6,30),GAS(6),Z(30),Z(30)	FI 1A0210
00104	3.	DIMENSION	FC(30),FCS(30),FV(30),Z(30),V(30)	FI 1A0210
00105	4.	COMMON	SI(40),LC,IR,NTOT,NCS1,NCS2,EXT	FI 1A0230
00106	5.	DO	10 J=1,IR	FI 1A0230
00111	6.	FCS(J)=0.		FI 1A0230
00112	7.	DO	11 K=1,LC	FI 1A0230
00115	8.	11 FCS(J)=FCS(J)+AVCON(K,J)		FI 1A0230
00117	9.	10 CONTINUE		FI 1A0230
00121	10.	GT=0.		FI 1A0230
00122	11.	DO	20 L=1,LC	FI 1A0230
00125	12.	20 GT=GT+GAS(L)		FI 1A0230
00127	13.	VFE0.		FI 1A0230
00130	14.	DO	30 K=1,IR	FI 1A0230
00133	15.	Z(K)=Z(1)+V(K)		FI 1A0230
00134	16.	V(K)=Z(K)+V(K)		FI 1A0230
00135	17.	30 VFE0=V(K)		FI 1A0230
00137	18.	DO	40 I=1,IR	FI 1A0230
00142	19.	FC(I)=Z(I)+G(I)+VFE0		FI 1A0230

00143	20.	40 F4(I)=FC(I)*T(I)	FI A0650
00143	21.	C	FI A0700
00143	22.	C	FI A0710
00143	23.	C	FI A0720
00145	24.	WRITE(6,100)NAME,ICS1,ICS2,NAME	FI A0730
00153	25.	DO 50 K=1,IR	FI A0740
00156	26.	50 WRITE(6,101)R(K),FCS(K),FC(K),FY(K)	FI A0750
00165	27.	RETURN	FI A0760
00166	28.	100 FOR K1=(M1-47X+22+LOW3-TERM RESULTS FOR 24.6CM ISOTOPE,16X,9MCASE	FI A0770
00166	29.	..N0.,.13,14.,.A47/9X,.15+PARTICLE RADIUS,.9X,21+WAVELENGTH CONCENTRATION,0.1	FI A0780
00166	30.	..5X,27+TOTAL AVERAGE CONCENTRATION,0.5X,15+TOTAL AMOUNT OF 24.6CM ISOTOPE	FI A0790
00166	31.	..12X,20+DUE TO SOLID'S DECAY,.5X,25+H1+CLONES GAS PHASE,0.6X,20,1X,1E1	FI A0800
00166	32.	..24 IN PARTICLE/36X,7H(47/54),22X,7H(67/54),20X,4H(41)	FI A0810
00167	33.	101 FORMAT(13X,F7.5,12X,1PE14.3,15X,1PE14.3,13X,1PE16.6)	FI A0820
00170	34.	END	FI A0830

END OF LISTING. 0 DIAGNOSTIC MESSAGE(S).

SUBROUTINE BCALC

01 FOR BCALC
 COMPILATION BY UNIVAC 1106 FORTRAN-IV DATED 11 NOV 1966 F4008
 THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:06:12

SUBROUTINE BCALC ENTRY POINT 000157

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CCL 000225
 0000 *DATA 000030
 0002 *BLANK 001676
 0003 SING 000005
 0004 BI 023160
 0005 INLOOP 000001

EXTERNAL REFERENCES (BLOCK, NAME)

0006 DIFFUS

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000116	11L	0001	000110	12L	0001	000043	1315	0001	000131	1003	0001	000027	20L
0001	000153	30C	0001	000027	30L	0002	001134	AK	0002	001025	ATM	0003	000030	30V
0002	R	000374	DIFFUS	0006	R	000000	EMISL	0002	000754	HEI	0003	I	000001	30
0000	I	000002	J	0000	I	000010	K	0005	I	000000	L	0003	I	000005
0002	000360	NAME	0003	000003	NCS1	0003	000004	NCS2	0000	I	000003	REL	0003	I
0000	I	000011	MSG	0003	000002	NTOT	0000	I	000005	SI	0002	R	001342	3
0000	R	000001	SVSU4	0002	R	001546	T	0002	001556	TEMP	0002	001436	YCL	0002
0004	022600	BI	0002	R	001800	YT	0002	000000	YLN					0002

00101 1. SUBROUTINE BCALC(N,T,I,KLAG,S,DD,DT)
 00101 2. C SUBROUTINE TO CALCULATE SOLUTIONS TO THE DIFFUSION EQUATION.
 00101 3. C FIRST SECTION COMPUTES THE PROPER DT VALUE.
 00103 4. DIMENSION ITG)
 00104 5. COMMON YLD(5,40),IA,E(6),XVOL(6),DEC(6,40),MEI(6,40),AK(6),R(30),T
 00104 6. /T(30),VOL(40),T(40),TEMP(40),AT(40)
 00105 7. COMMON/SING/LC,IR,NTOT,NCS1,NCS2
 00106 8. COMMON/BI/BCY(6,40),ZOT/ZN(6,40)
 00107 9. COMMON/INLOOP/L
 00110 10. DIMENSION DD(11)
 00111 11. DATA EPISLN/.0001/
 00113 12. SVSU=0
 00114 13. J=3
 00115 14. NEL=N
 00116 15. SUM=0
 00117 16. NIEN=IT(1)

SUBROUTINE BCALC

Q1 FOR BCALC
 COMPILE BY UNIVAC 1106 FORTRAN-IV DATED 11 NOV 1966 F#005
 THIS COMPILE WAS DONE ON 19 DEC 66 AT 21:06:12

SUBROUTINE BCALC ENTRY POINT 000157

STORAGE USED (BLOCK, NAME, LENGTH)

0001	*CODE	000225
0000	*DATA	000030
0002	*BLANK	001676
0003	SING	000005
0004	BI	023160
0005	INLOOP	000001

EXTERNAL REFERENCES (BLOCK, NAME)

0006 DIFFUS

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000116	11L	0001	000110	12L	0001	000043	131S	0001	000131	100J	0001	000027	20L				
0001	000153	30L	0001	000067	20L	0002	001334	AK	0002	001025	AY	0003	000003	2CV				
0002	R	000374	LFC	0006	R	000000	DIFFUS		0000	R	000000	EPISLN	0003	I	000001	10		
0000	I	000002	J	0000	I	000010	K		0005	I	000000	L	0003	I	000005	10		
0002	000360	NAME	0003	000003	1CS1	0003	000004	NC52	0000	I	000003	DEL	0003	I	000007	200		
0000	I	000011	NC5	0003	000002	1TOT	0000	I	000005	11	0002	R	001342	2	0003	R	000004	510
0000	M	000001	SVSU4	0002	M	001506	1		0002	001556	TEMP	0002	001436	2CL	0002	000365	200L	
0004	022600	BI	0002	R	001800	11	0002	000000	YLN									

00101 1. SUBROUTINE BCALC(N,IT,I,KL,AG,9,DD,DT)
 00101 2. C SUBROUTINE TO CALCULATE SOLUTIONS TO THE DIFFUSION EQUATION.
 00101 3. C FIRST SECTION COMPUTES THE PROPER DT VALUE.

00103 4. DIMENSION I(6)
 00104 5. COMMON YLD(5,40),IA,E(6),AQL(6),DEC(6,40),HEI(6,40),AK(a),X(30),Y
 00105 6. /T(30),VOL(40),T(40),TEMP(40),ATHT(40)
 00106 7. COMMON/SING/LC,IR,1TOT,NC51,NC52
 00107 8. COMMON/BI/DTY(6,40,20),HIT(6,40)
 00107 9. COMMON/INLOOP/L
 00110 10. DIMENSION DUT(1)
 00111 11. DATA EPISLN/.0001/
 00113 12. SVSU=0
 00114 13. J=3
 00115 14. NEL=0
 00116 15. SUM=0
 00117 16. NIT=0-1(1)

00120	17.	M1=1+1(2)+1
00121	18.	IF(KLAG)50,50,20
00124	19.	50 M1=M1+1
00125	20.	IF(M1-GT-M1)GO TO 60
00127	21.	20 NEP=NEL+L-1
00130	22.	DO 10 K=M1,M1
00133	23.	SUM=SUM+DFC(NEP,K)*I(K)
00134	24.	IF(ABS(SVSUM-SUM).LT.ABS(EPI*SUM-SVSUM)) GO TO 11
00136	25.	S/SUM=SUM
00137	26.	10 CONTINUE
00141	27.	60 NEL=NEL-1
00142	28.	IF(NEL-1)11,12,13
00145	29.	13 M1=M1+1
00146	30.	M1=M1+1(J)+1
00147	31.	J=J+1
00150	32.	GO TO 20
00151	33.	12 M1=M1+1
00152	34.	M1=M1
00153	35.	GO TO 20
00154	36.	11 DT=SUM
00155	37.	SUM=0
00156	38.	NCG=M1-I(1)+1
00157	39.	DO 30 K=1,IR
00162	40.	DJ(K)=1,0
00163	DIAGNOSTIC*	THE TEST FOR EQUALITY BETWEEN NON-INTegers MAY NOT BE MEANINGFUL.
00163	41.	IF(DTGE*(1-DB(K)*2))GO TO 30
00165	42.	DJ(K)=DIFFUS(DT,R(K))
00166	43.	30 SUM=SUM+DJ(K)*DT(K)
00170	44.	B=SUM
00171	45.	RETURN
00172	46.	END

END OF LISTING. 1 *DIAGNOSTIC* MESSAGE(S).

SUBROUTINE DELTA

01 FOR DELTA
 COMPILATION BY UNIVAC 1100 FORTRAN-IV DATED 11 NOV 1966 F0009
 THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:06:15

SUBROUTINE DELTA ENTRY POINT 000172

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CODE 000221
 0000 *DATA 000043
 0002 *BLANK 000000
 0003 B1 023160
 0004 I-LOOP 000001

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001 000111 IOL 0001 000021 I106 0001 000052 I2L 0001 000084 I203 0001 000127 I206
 0001 000156 I536 0001 000152 I7L 0003 R 000000 DCY 0000 R 000000 DELT 0000 R 000016 PLT
 0000 I 000011 ISUM 0000 I 000007 J 0000 I 000012 K 0004 I 000000 L 0000 I 000010 M
 0000 I 000013 N02 0000 I 000014 N03 0000 I 000015 N04 0000 I 000006 NE 0003 000000 NY

00101 1. SUBROUTINE DELTA(NIT, IOPR)
 00103 2. DIMENSION I(6), DELT(6)
 00104 3. COMMON/317DCY(6*0,0), ZN(6*0)
 00105 4. COMMON/I-LOOP/L
 00106 5. NEER=1
 00107 6. DO 10 J=1, NE
 00112 7. N01=N-J*L
 00113 8. ISUM=I-1(1)
 00114 9. IF(J=1) I1, I2, I1
 00117 10. 11 DO 14 K=2, J
 00122 11. 14 ISUM=ISUM+I(K)
 00124 12. ISUM=ISUM+2*J-2
 00125 13. 12 N02=ISUM
 00126 14. N03=ISUM+1(J+1)
 00130 15. N04=N03*1
 00130 16. DELT=1.
 00131 17. IF((N03*LE.0).OR.(N02*LE.0)760 TO 10
 00133 18. DELT=DCY(N01, N02, N03)
 00134 19. 10 DELT(J)=DELT(I-DCY(N01, N02, N03))
 00136 20. ISUM=I-1(1)
 00137 21. DO 15 K=2, N
 00142 22. 15 ISUM=ISUM+I(K)
 00144 23. ISUM=ISUM+2*NE
 00145 24. DELT(N)=1.
 00146 25. IF((ISUM*LE.0)60 TO 17
 00150 26. DELT(N)=DCY(L, ISUM, NIT-1)
 00151 27. 17 PREL.

SUBROUTINE DELTA

00152 28. 00 10 K10N
00155 29. 10 PREPR*DELTA(K)
00157 30. RETURN
00160 31. END

END OF LISTING. 0 *DIAGNOSTIC* MESSAGE(S).

FUNCTION DIFFUS

01 FOR DIFFUS
 COMPILE BY UNIVAC 1108 FORTRAN-IV DATED 11 NOV 1966 F#009
 THIS COMPILE HAS DONE ON 19 DEC 66 AT 21:06:18

FUNCTION DIFFUS ENTRY POINT 000000

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CODE 000066
 0000 *DATA 000021
 0002 *BLANK 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 SORT
 0004 EXP

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001 000021 10L 0001 000020 12L 0000 000001 CONST 0000 000002 C1 0000 000003 C2
 0000 R 000000 DIFFUS 0000 R 000000 EXP 0000 R 000000 SUP 0000 R 000000 X 0000 R 000000 Y

00101 1. FUNCTION DIFFUS(OT,R)
 00103 2. DATA CONST,C1,C2/1.128379,.60792710,-9.4596044/
 00107 3. X=R/SORT(OT)
 00110 4. IF(X-3.141592653589793)10,20
 00113 5. 20 DIFFUS=3.*(CONST-1./4)/X
 00114 6. 12 RETURN
 00115 7. 10 Y=X**2
 00116 8. DIFFUS=1.-C1*EXP(C2/Y)
 00117 9. IF(X-2.)12,12.15
 00122 10. 15 DIFFUS=DIFFUS-C1*EXP(C2/Y)/Y.
 00123 11. RETURN
 00124 12. END

END OF LISTING. 0 *DIAGNOSTIC MESSAGE(S).

FUNCTION PROFILE

01 FOR PROFIL

COMPILATION BY UNIVAC 1108 FORTRAN-IV DATED 11 NOV 1966 F4004
THIS COMPILATION WAS DONE ON 19 DEC 66 AT 21:06:20

FUNCTION PROFILE ENTRY POINT 000342

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CLOC 000350
0000 *DATA 000043
0002 *BLANK 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 SIN
0004 EXP
0005 SINT
0006 ERF
0007 HEXPIS

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0001	000031	10L	0001	000014	20L	0001	000135	21L	0001	000231	30L	0001	000253	30L
0001	000330	32L	0001	000146	40L	0001	000151	41L	0001	000224	42L	0001	000297	50L
0001	000307	3L	0000	R	000000	01	0000	000001	01R	0003	000300	50F	0003	000303
0000	I	000012	1S	0000	I	000014	J	0000	I	000015	1L	0003	000311	3750
0000	R	000000	PROFIL	0000	R	000017	PSUM	0000	R	000013	R	0003	000300	51L
0000	R	000016	SUM									0003	000300	54L

00101 1. C FUNCTION PROFILE(101,172)

00101 2. C

00101 3. C FUNCTION COMPUTES CONCENTRATION AT RAD. Z-A FOR SPHERICAL

00101 4. C PARTICLE OF RADIUS A.

00101 5. C

00103 6. C DIMENSION DT(17)

00104 7. DATA PI/3.1415926/.015079.8586044/.075/1..1..001..000001..00000000

00104 8. .000001.1.E-9/

00110 *DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTEGER VALUES MAY NOT BE MEANTINGFUL.

00110 9. IF(2.E0.0)GO TO 40

00112 10. RZ=0

00113 11. J=0

00114 *DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTEGER VALUES MAY NOT BE MEANTINGFUL.

00114 12. 9 IF(A(10..J).SE.(.99)) GO TO 10

00116 13. J=J+1

00117 14. GO TO 9

00120 15. 10 IF(DT.LY.DT(BJ.0))GO TO 30

000F0010
000F0020
000F0030
000F0040
000F0050
000F0060
000F0070
000F0080
000F0090
000F0100
000F0110
000F0120
000F0130
000F0140
000F0150
000F0160
000F0170
000F0180
000F0190
000F0200
000F0210
000F0220
000F0230
000F0240
000F0250
000F0260
000F0270
000F0280
000F0290
000F0300
000F0310
000F0320
000F0330
000F0340

FUNCTION PROFIL

00122	16.	N=1	PROF0350
00123	17.	SUM=0.	PROF0350
00124	18.	20 PSUM=SUM	PROF0350
00125	19.	SUM=SUM+((-1)*PI*27A)*EXP((-2)*PI*27A*PI*50/(A**2)))/PI	PROF0350
00126	DIAGNOSTIC	THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE NEARLY SUFF.	
00127	20.	IF (ABS(SUM-PSUM).LE.(1.E-2)*ABS(SUM)) GO TO 21	
00128	21.	N=N+1	PROF0350
00129	22.	IF (N-100)20*20*21	PROF0350
00130	23.	21 PROFIL=1.+(2.*PI*27A)*SUM	PROF0350
00131	24.	RETURN	PROF0350
00132	25.	40 N=1	PROF0350
00133	26.	SUM=0.	PROF0350
00134	27.	41 PSUM=SUM	PROF0350
00135	28.	SUM=SUM+((-1)*PI*27A)*EXP((-2)*PI*27A*PI*50/(A**2))	PROF0350
00136	DIAGNOSTIC	THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE NEARLY SUFF.	
00137	29.	IF (ABS(SUM-PSUM).LE.(1.E-2)*ABS(SUM)) GO TO 30	
00138	30.	N=N+1	PROF0350
00139	31.	IF (N-100)41*41*42	PROF0350
00140	32.	42 PROFIL=1.+(2.*PI*27A)*SUM	PROF0350
00141	33.	RETURN	PROF0350
00142	34.	C	PROF0350
00143	35.	C	PROF0350
00144	36.	C	PROF0350
00145	37.	30 CIE1/12.*SUM*PI*PI	PROF0350
00146	DIAGNOSTIC	THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE NEARLY SUFF.	
00147	38.	IF ((A-RT)*C1.CE.3.5)*50 TO 60	PROF0350
00148	39.	SUM=0.	PROF0350
00149	40.	N=0	PROF0350
00150	41.	31 PSUM=SUM	PROF0350
00151	42.	SUM=SUM+((-1)*PI*27A)*EXP((-2)*PI*27A*PI*50/(A**2))	PROF0350
00152	DIAGNOSTIC	THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE NEARLY SUFF.	
00153	43.	IF (ABS(SUM-PSUM).LE.(1.E-2)*ABS(SUM)) GO TO 32	PROF0350
00154	44.	N=N+1	PROF0350
00155	45.	IF (N-100)31*31*32	PROF0350
00156	46.	32 PROFIL=1.+(2.*PI*27A)*SUM	PROF0350
00157	47.	RETURN	PROF0350
00158	48.	E.O	PROF0350
00159	49.		PROF0350

END OF LISTING. 6 *DIAGNOSTIC* MESSAGE(S).

FUNCTION ERF

01 FOR ERF
 COMPILE BY UNIVAC 1105 FORTRAN-IV DATED 11 NOV 1956 F4008
 THIS COMPILE HAS DME JN 19 DEC 66 AT 21:06:23

FUNCTION ERF ENTRY POINT 000050

STORAGE USED (BLOCK, NAME, LENGTH)

0001 *CODE 300034
 0000 *DATA 000013
 0002 *BLANK 000000

EXTERNAL REFERENCES (BLOCK, NAME)

0003 EXP

STORAGE ASSIGNMENT FOR VARIABLES (BLOCK, TYPE, RELATIVE LOCATION, NAME)

0000 R 000000 ERF 0003 R 000030 EXP 0000 R 000001 Y

00101 1. FUNCTION ERF(X)

00101	1.	FUNCTION ERF(X)	ERF	0010
00101	2.	C		0020
00101	3.	C	COMPUTES ERROR FUNCTION WITH AN ERROR OF LESS THAN 2.5E-5.	0030
00101	4.	C	SEE HANDBOOK OF MATH. FUNCTIONS WITH FORMULAS, GRAPHS AND TABLES.	0040
00101	5.	C	TABLES, MARCH 1955. NBS APPLIED MATHEMATICS SERIES 55, PAGE 294	0050
00101	6.	C	PARAGRAPH 7.1.25.	0060
00101	7.	C		0070
00103	8.	Y=1.711+.47067EX		0080
00104	9.	ERF=1.-T*(.3480242+T*(.09513798+T*(.7478556))) *EXP(-X**2)		0090
00105	10.	RETURN		0100
00106	11.	END		0110

END OF LISTING. 0 *DIAGNOSTIC MESSAGE(S).

FUNCTION MARGIN

CALL	ASM	MARGIN	THIS SUBROUTINE ASSIGNS THE LOCATION OF THE FIRST AND LAST LINE TO TO PRINTED	CALL MAPS TO TOP BOTTOM MESSAGE	NUMBER OF BLANK LINES ON TOP OF THE PAGE LAST LINE TO BE PRINTED
000001	01	000000	00 00 13 00 0 000011	SA	5110011
000002			20-35 +CC 1	LA	5110011
000003			000001 10 00 00 13 1 000000	SA	5110011
000004			000002 01 06 00 00 0 000006	SA	5110011
000005			20-35 +CC 1	LA	5110011
000006			000003 10 00 00 13 1 000001	SA	5110011
000007			000004 01 05 00 00 0 000006	SA	5110011
000008			20-35 +CC 1	LA	5110011
000009			000005 74 13 13 00 0 001030	LA	5110011
000010			000006 0102 0000 0000	LA	5110011
000011			000007 27 00 13 00 0 000011	LA	5110011
000012			20-35 +CC 1	LA	5110011
000013			000010 74 04 00 13 0 000003	LA	5110011
000014			000011 000000000000	LA	5110011
000015				LA	5110011
000016				LA	5110011
000017				LA	5110011
000018				LA	5110011
000019				LA	5110011

REFERENCES

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2. Crocker, G. R., "Estimates of Fission Product Yields of a Thermo-nuclear Explosion," U.S. Naval Radiological Defense Laboratory Report USNRDL-TR-642, 1963.
3. Crocker, G. R., R. C. Scheidt, and M. D. Connors, "Radionuclide Input Data for Fission Product Abundance Computations," U.S. Naval Radiological Defense Laboratory Report USNRDL-TM-137, 1963.
4. Norman, J. H., "Henry's Law Constants for Dissolution of Fission Products in a Silicate Fallout Particle Matrix," U.S. Naval Radiological Defense Laboratory Report GA-7058, General Atomic Division, General Dynamics Corporation, November 1966.
5. Crank, J., Mathematics of Diffusion, Oxford University Press, London, 1956.

DOCUMENT CONTROL DATA - R&D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) General Atomic Division General Dynamics Corporation San Diego, California		2a. REPORT SECURITY CLASSIFICATION Unclassified	
		2b. GROUP	
3. REPORT TITLE A CALCULATIONAL MODEL FOR CONDENSED STATE DIFFUSION CONTROLLED FISSION PRODUCT ABSORPTION DURING FALLOUT FORMATION			
4. DESCRIPTIVE NOTES (Type of report and inclusive dates)			
5. AUTHOR(S) (Last name, first name, initial) Korts, Richard F. and Norman, John H.			
6. REPORT DATE January 10, 1967		7a. TOTAL NO. OF PAGES 91	7b. NO. OF REFS 5
8a. CONTRACT OR GRANT NO. N0022866C0403		8a. ORIGINATOR'S REPORT NUMBER(S) GA-7598	
b. PROJECT NO.			
c.		9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)	
d.			
10. AVAILABILITY/LIMITATION NOTICES Distribution of this document is unlimited			
11. SUPPLEMENTARY NOTES		12. SPONSORING MILITARY ACTIVITY Office of the Civil Defense, Office of the Secretary of the Army, Washington, D.C. 20310	
13. ABSTRACT A program is presented to compute fallout fission product absorption in an expanding, cooling, uniform field of gas and fallout particles where the rate of fission product absorption is controlled by fission product surface concentrations as given by Henry's law constants and diffusion of these fission products into the fallout particles. The calculations are made a nuclide chain at a time, employing nuclear device and fission product parameters. Program output includes average concentration versus particle size for each absorbed fission product at a pre-selected lower temperature and the amount of that fission product in the gas phase, with an option for the calculation of fission product radial profiles versus particle size.			

UNCLASSIFIED
Security Classification

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Surface concentration Concentration profiles Fallout formation Fission products Absorption Diffusion						

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